Docket/App No.: 2079.1037-001

Title: Method of Identifying Inhibitors of TIE-2 Inventors: Nancy J. Bump *et al.*

MDSLASLVLC GVSLLLSGTV EGAMDLILIN SLPLVSDAET SLTCIASGWR PHEPITIGRD FEALMNQHQD PLEVTQDVTR EWAKKVVWKR EKASKINGAY FCEGRVRGEA IRIRTMKMRO QASFLPATLT MTVDKGDNVN ISFKKVLIKE EDAVIYKNGS FIHSVPRHEV PDILEVHLPH AQPQDAGVYS ARYIGGNLFT SAFTRLIVRR CEAQKWGPEC NHLCTACMNN GVCHEDTGEC ICPPGFMGRT CEKACELHTF GRTCKERCSG QEGCKSYVFC LPDPYGCSCA TGWKGLQCNE ACHPGFYGPD CKLRCSCNNG EMCDRFQGCL CSPGWQGLQC EREGIPRMTP KIVDLPDHIE VNSGKFNPIC KASGWPLPTN EEMTLVKPDG TVLHPKDFNH TDHFSVAIFT IHRILPPDSG VWVCSVNTVA GMVEKPFNIS VKVLPKPLNA PNVIDTGHNF AVINISSEPY FGDGPIKSKK LLYKPVNHYE AWQHIQVTNE IVTLNYLEPR TEYELCVQLV RRGEGGEGHP GPVRRFTTAS IGLPPPRGLN LLPKSQTTLN LTWQPIFPSS EDDFYVEVER RSVQKSDQQN IKVPGNLTSV LLNNLHPREQ YVVRARVNTK AQGEWSEDLT AWTLSDILPP QPENIKISNI THSSAVISWT ILDGYSISSI TIRYKVQGKN EDQHVDVKIK NATIIQYQLK GLEPETAYQV DIFAENNIGS SNPAFSHELV TLPESQAPAD LGGGKMLLIA ILGSAGMTCL TVLLAFLIIL QLKRANVQRR MAQAFQNVRE EPAVQFNSGT LALNRKVKNN PDPTIYPVLD WNDIKFQDVI GEGNFGQVLK ARIKKDGLRM DAAIKRMKEY ASKDDHRDFA GELEVLCKLG HHPNIINLLG ACEHRGYLYL AIEYAPHGNL LDFLRKSRVL ETDPAFAIAN STASTLSSQQ LLHFAADVAR GMDYLSQKQF IHRDLAARNI LVGENYVAKI ADFGLSRGQE VYVKKTMGRL PVRWMAIESL NYSVYTTNSD VWSYGVLLWE IVSLGGTPYC GMTCAELYEK LPQGYRLEKP LNCDDEVYDL MRQCWREKPY ERPSFAQILV SLNRMLEERK TYVNTTLYEK FTYAGIDCSA EEAA

FIG. 1

ALNRKVKNN	PDPTIYPVLD	WNDIKFQDVI	GEGNFGQVLK
ARIKKDGLRM	DAAIKRMKEY	ASKDDHRDFA	GELEVLCKLG
HHPNIINLLG	ACEHRGYLYL	AIEYAPHGNL	LDFLRKSRVL
ETDPAFAIAN	STASTLSSQQ	LLHFAADVAR	GMDYLSQKQF
IHR N LAARNI	LVGENYVAKI	ADFGLSRGQE	VYVKKTMGRL
PVRWMAIESL	NYSVYTTNSD	VWSYGVLLWE	IVSLGGTPYC
GMTCAELYEK	LPQGYRLEKP	LNCDDEVYDL	MRQCWREKPY
ERPSFAQILV	SLNRMLEERK	TYVNTTLYEK	FTYAGIDCSA
EEAA			

) 2079.1037-001
Title: Method of	f Identifying Inhibitors of TIE-2
Inventors:	Nancy J. Bump et al.

	CRYST1	95	.604	117	.589 78.2	14 90.0	0 90.00	90.00		
	ORIGX1		1.000	0000	0.000000	0.00000	0	0.00000		
	ORIGX2		0.000	0000	1.000000	0.00000	0	0.00000		
	ORIGX3		0.000	0000	0.000000	1.00000	0	0.00000		
	SCALE1		0.01	0460	0.000000	0.00000	0	0.00000		
	SCALE2		0.000	0000	0.008504	0.00000	0	0.00000		
	SCALE3		0.000	0000	0.000000	0.01278	5	0.00000		
	ATOM	1	CB	VAL	818	5.159	51.390	-17.822	1.00 65.41	6
	ATOM	2	C	VAL	818	3.553	51.091	-15.926	1.00 99.70	6
	ATOM	3	0	VAL	818	2.603	51.682	-16.444	1.00 99.70	8
	ATOM	4	N	VAL	818	4.074	49.203	-17.428	1.00 99.70	7
	ATOM	5	CA	VAL	818	4.628	50.419	-16.774	1.00 99.70	6
	ATOM	6	N	LEU	819	3.729	50.991	-14.616	1.00100.00	7
	ATOM	7	CA	LEU	819	2.912	51.555	-13.639	1.00100.00	6
	ATOM	8	CB	LEU	819	3.310	51.175	-12.250	1.00 77.77	6
	ATOM	9	CG	LEU	819	2.625	51.796	-11.045	1.00 67.90	6
	ATOM	10	CD1	LEU	819	1.161	51.416	-11.022	1.00 67.90	6
	ATOM	11	CD2	LEU	819	3.336	51.313	-9.810	1.00 67.90	б
	ATOM	12	C	LEU	819	2.607	53.076	-13.729	1.00100.00	6
	ATOM	13	0	LEU	819	3.568	53.838	~13.899	1.00100.00	8
	ATOM	14	N	ASP	820	1.351	53.507	-13.602	1.00100.00	7
	ATOM	15	CA	ASP	820	0.990	54.928	-13.659	1.00100.00	6
	ATOM	16	CB	ASP	820	-0.505	55.084	-13.929	1.00100.00	6
	ATOM	17	CG	ASP	820	-0.910	56.525	-14.140	1.00100.00	6
10	ATOM	18	OD1	ASP	820	-2.054	56.874	-13.785	1.00100.00	8
(1)	ATOM	19	OD2	ASP	820	-0.087	57.303	-14.663	1.00100.00	8
	ATOM	20	С	ASP	820	1.314	55.593	-12.329	1.00100.00	б
1,39	ATOM	21	0	ASP	820	0.786	55.200	-11.290	1.00100.00	8
1.1	ATOM	22	N	TRP	821	2.171	56.605	-12.361	1.00100.00	7
.00	ATOM	23	CA	TRP	821	2.558	57.278	-11.132	1.00100.00	6
Section	ATOM	24	CB	TRP	821	3.291	58.582	-11.458	1.00 96.30	6
	ATOM	25	CG	TRP	821	3.985	59.118	-10.263	1.00 96.04	6
390	ATOM ATOM	26	CD2	TRP	821	3.369	59.782	-9.149	1.00 96.04	6
1.1	ATOM	27	CE2	TRP	821	4.371	59.991	-8.185	1.00 96.04	6
14	ATOM	28	CE3	TRP	821	2.061	60.200	-8.869	1.00 96.04	6
N	ATOM	29	CD1	TRP	821	5.302	58.974	-9.938	1.00 96.04	6
10	ATOM	30	NE1	TRP	821	5.545	59.494	-8.689	1.00 96.04	7
63	ATOM	31	CZ2	TRP	821	4.106	60.614	-6.976	1.00 96.04	6
3.15	ATOM	32	CZ3	TRP	821	1.803	60.816	-7.657	1.00 96.04	6
	ATOM	33	CH2	TRP	821	2.824	61.007	-6.733	1.00 96.04	6
	ATOM	34	C	TRP	821	1.355	57.543	-10.207	1.00100.00	6
	ATOM	35	0	TRP	821	1.462	57.434	-8.983	1.00100.00	8
	ATOM	36	N	ASN	822	0.207	57.853	-10.801	1.00 78.55	7
	ATOM	37	CA	ASN	822	-1.018	58.149	-10.061	1.00 78.55	6
	ATOM	38	CB	ASN	822	-2.158	58.380	-11.037	1.00100.00	6
	ATOM	39	CG	ASN	822	-3.126	59.416	-10.546	1.00100.00	6
	ATOM	40	OD1	ASN	822	-3.508	60.321	-11.291	1.00100.00	8
	MOTA	41	ND2	ASN	822	-3.536	59.303	-9.286	1.00100.00	7
	ATOM	42	C	ASN	822	-1.453	57.094	-9.048	1.00 78.55	6
	MOTA	43	0	ASN	822	-1.451	57.340	-7.842	1.00 78.55	8
	ATOM	44	N	ASP	823	-1.854	55.933	-9.554	1.00 95.03	7
	ATOM	45	CA	ASP	823	-2.308	54.841	-8.704	1.00 95.03	6
	ATOM	46	CB	ASP	823	-2.991	53.775	-9.562	1.00 65.89	6
	ATOM	47	C	ASP	823	-1.158	54.218	-7.916	1.00 95.03	6

ATOM	48	0	ASP	823	-0.967	53.008	-7.949	1.00 95.03	8
ATOM	49	N	ILE	824	-0.384	55.043	-7.221	1.00 88.67	7
ATOM	50	CA	ILE	824	0.729	54.531	-6.426	1.00 88.67	6
ATOM	51	CB	ILE	824	2.112	54.819	-7.082	1.00 53.67	6
ATOM	52	CG2	ILE	824	3.202	54.080	-6.326	1.00 56.64	6
ATOM	53	CG1	ILE	824	2.161	54.314	-8.526	1.00 56.64	6
ATOM	54	CD1	ILE	824	3.503	54.615	-9.196	1.00 56.64	6
ATOM	55	C	ILE	824	0.701	55.176	-5.041	1.00 88.67	6
ATOM	56	0	ILE	824	1.617	55.912	-4.665	1.00 88.67	8
ATOM	57	N	LYS	825	-0.361	54.889	-4.292	1.00 65.97	7
ATOM	58	CA	LYS	825	-0.552	55.426	-2.947	1.00 65.97	6
ATOM	59	CB	LYS	825	-1.917	54.995	-2.406	1.00 30.30	6
ATOM	60	C	LYS	825	0.544	55.003	-1.973	1.00 65.97	6
ATOM	61	0	LYS	825	0.502	53.909	-1.401	1.00 65.97	8
ATOM	62	N	PHE	826	1.526	55.879	-1.788	1.00 96.52	7
ATOM	63	CA	PHE	826	2.632	55.608	-0.878	1.00 96.52	6
ATOM	64	CB	PHE	826	3.784	56.586	-1.112	1.00 96.59	6
MOTA	65	CG	PHE	826	4.397	56.474	-2.463	1.00100.00	6
MOTA	66	CD1	PHE	826	3.989	57.310	-3.489	1.00100.00	6
ATOM	67	CD2	PHE	826	5.351	55.500	-2.726	1.00100.00	6
MOTA	68	CE1	PHE	826	4.518	57.181	-4.764	1.00100.00	6
ATOM	69	CE2	PHE	826	5.888	55.358	-4.001	1.00100.00	6
ATOM	70	CZ	PHE	826	5.469	56.202	-5.023	1.00100.00	6
ATOM	71	C	PHE	826	2.158	55.727	0.565	1.00 96.52	6
ATOM	72	0	PHE	826	1.746	56.794	0.991	1.00 96.52	8
MOTA	73	N	GLN	827	2.247	54.651	1.332	1.00100.00	7
ATOM	74	CA	GLN	827	1.769	54.708	2.698	1.00100.00	6
ATOM	75	CB	GLN	827	0.886	53.484	2.937	1.00100.00	6
ATOM	76	CG	GLN	827	-0.252	53.407	1.903	1.00100.00	6
ATOM	77	CD	GLN	827	~1.539	52.860	2.488	1.00100.00	6
MOTA	78	OE1	GLN	827	-1.553	51.771	3.060	1.00100.00	8
ATOM	79	NE2	GLN	827	-2.633	53.615	2.349	1.00100.00	7
ATOM	80	C	GLN	827	2.840	54.886	3.781	1.00100.00	6
ATOM	81	0	GLN	827	2.892	55.942	4.395	1.00100.00	8
ATOM	82	N	ASP	828	3.696	53.894	4.015	1.00 99.72	7
MOTA	83	CA	ASP	828	4.713	54.034	5.064	1.00 99.72	6
ATOM	84	CB	ASP	828	4.144	53.510	6.388	1.00 87.03	6
ATOM	85	CG	ASP	828	5.121	53.627	7.533	1.00 84.60	6
ATOM	86	OD1	ASP	828	5.870	54.617	7.572	1.00 84.60	8
ATOM	87	OD2	ASP	828	5.128	52.740	8.406	1.00 84.60	8
ATOM	88	C	ASP	828	6.003	53.286	4.720	1.00 99.72	6
ATOM	89	0	ASP	828	5.961	52.262	4.034	1.00 99.72	8
ATOM	90	N	VAL	829	7.154	53.772	5.178	1.00 85.45	7
ATOM	91	CA	VAL	829	8.408	53.075	4.863	1.00 85.45	6
ATOM	92	CB	VAL	829	9.606	53.874	5.391	1.00 51.35	6
ATOM	93	C	VAL	829	8.460	51.633	5.402	1.00 85.45	6
MOTA	94	0	VAL	829	8.437	51.418	6.615	1.00 85.45	8
ATOM	95	N	ILE	830	8.538	50.663	4.488	1.00100.00	7
ATOM	96	CA	ILE	830	8.598	49.244	4.852	1.00100.00	6
MOTA	97	CB	ILE	830	8.745	48.326	3.602	1.00100.00	6
ATOM	98	CG2	ILE	830	9.458	47.031	3.973	1.00 81.07	6
MOTA	99	CG1	ILE	830	7.370	48.034	2.994	1.00 81.07	6
ATOM	100	CD1	. ILE	830	6.385	47.414	3.969	1.00 81.07	6
ATOM	101	C	ILE	830	9.788	49.013	5.769	1.00100.00	6
ATOM	102	0	ILE	830	9.782	48.103	6.596	1.00100.00	8
ATOM	103	N	GLY	831	10.821	49.834	5.605	1.00 95.79	7
ATOM	104	CA	GLY	831	11.992	49.713	6.453	1.00 95.79	6

ATOM	105	С	GLY	831	13.352	49.743	5.806	1.00 95.79	_
ATOM	106	ō	GLY	831	13.497	50.005	4.613	1.00 95.79	6 8
ATOM	107	N	GLU	832	14.357	49.480	6.630	1.00 99.78	7
ATOM	108	CA	GLU	832	15.760	49.427	6.231	1.00 99.78	6
ATOM	109	CB	GLU	832	16.055	48.055	5.602	1.00100.00	6
ATOM	110	CG	GLU	832	16.417	46.997	6.632	1.00100.00	6
ATOM	111	CD	GLU	832	17.103	47.598	7.859	1.00100.00	6
ATOM	112	OE1		832	16.380	48.153	8.721	1.00100.00	8
ATOM	113	OE2		832	18.352	47.535	7.943	1.00100.00	8
ATOM	114	C	GLU	832	16.376	50.502	5.339	1.00100.00	6
ATOM	115	ō	GLU	832	15.689	51.284	4.679	1.00 99.78	8
ATOM	116	N	GLY	833	17.708	50.501	5.333	1.00 99.78	7
ATOM	117	CA	GLY	833	18.494	51.424	4.536	1.00100.00	6
ATOM	118	c	GLY	833	19.580	50.682	3.756	1.00100.00	6
ATOM	119	ō	GLY	833	19.557	49.446	3.693	1.00100.00	8
ATOM	120	N	ASN	834	20.540	51.432	3.192	1.00100.00	7
ATOM	121	CA	ASN	834	21.643	50.854	2.407	1.00100.00	6
ATOM	122	CB	ASN	834	22.414	49.810	3.241	1.00100.00	6
ATOM	123	CG	ASN	834	23.700	49.360	2.579	1.00100.00	6
ATOM	124		ASN	834	23.727	49.066	1.387	1.00100.00	8
ATOM	125		ASN	834	24.778	49.302	3.354	1.00100.00	7
ATOM	126	C	ASN	834	21.094	50.179	1.149	1.00100.00	6
ATOM	127	0	ASN	834	20.299	49.228	1.240	1.00100.00	8
ATOM	128	N	PHE	835	21.519	50.650	-0.030	1.00100.00	7
ATOM	129	CA	PHE	835	21.056	50.117	-1.328		
ATOM	130	CB	PHE	835	22.041	49.061	-1.328	1.00100.00	6
ATOM	131	CG	PHE	835	23.383	49.629	-2.294	1.00100.00	
ATOM	132	CD1	PHE	835	24.562	48.976	-1.954	1.00100.00	6
ATOM	133	CD2	PHE	835	23.465	50.835	-2.996	1.00100.00	6
ATOM	134		PHE	835	25.808	49.509	-2.291	1.00100.00	6
ATOM	135	CE2	PHE	835	24.706	51.380	-3.342	1.00100.00	6
ATOM	136	CZ	PHE	835	25.879	50.718	-2.987	1.00100.00	6
ATOM	137	c	PHE	835	19.641	49.519	-1.261	1.00100.00	6
ATOM	138	ō	PHE	835	19.380	48.467	-1.841	1.00100.00	8
ATOM	139	N	GLY	836	18.748	50.228	-0.570	1.00100.00	7
ATOM	140	CA	GLY	836	17.369	49.813	-0.397	1.00100.00	6
ATOM	141	C	GLY	836	16.689	50.596	0.720	1.00100.00	6
ATOM	142	0	GLY	836	17.188	50.622	1.840	1.00100.00	8
ATOM	143	N	GLN	837	15.571	51.261	0.418	1.00100.00	7
ATOM	144	CA	GLN	837	14.831	52.043	1.420	1.00100.00	6
ATOM	145	CB	GLN	837	15.333	53.505	1.420	1.00100.00	6
ATOM	146	CG	GLN	837	14.344	54.609	1.081	1.00100.00	6
ATOM	147	CD	GLN	837	15.041	55.948	0.852	1.00100.00	6
ATOM	148		GLN	837	15.798	56.108	-0.108	1.00100.00	8
ATOM	149		GLN	837	14.796	56.912	1.739	1.00100.00	7
ATOM	150	C	GLN	837	13.327	51.889	1.138	1.00100.00	6
ATOM	151	0	GLN	837	12.525	52.818		1.00100.00	
ATOM	152	N	VAL	838	12.993	50.652	1.236	1.00100.00	8 7
ATOM	153	CA	VAL	838	11.645	50.199			
ATOM	154	CB	VAL	838	11.565	48.683	0.469	1.00 49.78	6
ATOM	155	CG1	VAL	838	11.565	48.683	-0.703	1.00 54.51	6
ATOM	156	CG2	VAL	838	12.902	48.064	1.071	1.00 54.51	
ATOM	157	C	VAL	838	10.515	50.785		1.00 54.51	6
ATOM	158	0	VAL	838	10.515	50.785	1.303	1.00 49.78	6
ATOM	159	N	LEU	839	9.344	50.916			8
ATOM	160	CA	LEU	839	8.171	51.461	0.684 1.369	1.00 44.19	7 6
ATOM	161	CB	LEU	839	7.935	51.461	0.962		
	101	CD		000	7.935	52.921	0.962	1.00 90.21	6

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FIG. 3D

ATOM	219	CG	LEU	848	-6.201	44.560	-9.729	1.00 92.74	6
ATOM	220		LEU	848	-5.757	43.115	-9.491	1.00 92.74	6
ATOM	221	CD2	LEU	848	-6.753	44.595	-11.155	1.00 92.74	6
ATOM	222	c	LEU	848	-6.366	47.280	-7.954	1.00 86.45	6
ATOM	223	ō	LEU	848	-5.717	48.215	-8.445	1.00 86.45	8
ATOM	224	N	ARG	849	-6.211	46.809	-6.730	1.00 99.60	7
				849	-5.226	47.347	-5.780	1.00 99.60	6
ATOM	225	CA	ARG		-5.877	48.415	-4.899	1.00100.00	6
ATOM	226	CB	ARG	849			-5.692	1.00100.00	6
ATOM	227	CG	ARG	849	-6.736	49.403		1.00 99.93	6
ATOM	228	CD	ARG	849	-8.059	49.736	-4.998		7
ATOM	229	NE	ARG	849	-7.887	50.134	-3.594	1.00 99.93	
ATOM	230	CZ	ARG	849	-8.903	50.347	-2.746	1.00 99.93	6 7
MOTA	231		ARG	849	-10.175	50.205	-3.143	1.00 99.93	
ATOM	232	NH2	ARG	849	-8.747	50.710	-1.465	1.00 99.93	7
MOTA	233	C	ARG	849	-4.694	46.224	-4.887	1.00 99.60	6
ATOM	234	0	ARG	849	-5.398	45.242	-4.608	1.00 99.60	8
ATOM	235	N	MET	850	-3.457	46.411	-4.467	1.00 80.73	7
ATOM	236	CA	MET	850	-2.754	45.456	-3.599	1.00 80.73	6
MOTA	237	CB	MET	850	-1.967	44.457	-4.450	1.00100.00	6
ATOM	238	CG	MET	850	-2.734	43.994	-5.690	1.00 68.64	6
ATOM	239	SD	MET	850	-1.849	44.290	-7.206	1.00 68.64	16
ATOM	240	CE	MET	850	-0.189	43.661	-7.074	1.00 68.64	6
ATOM	241	c	MET	850	-1.782	46.199	-2.681	1.00 80.73	6
ATOM	242	ō	MET	850	-1.937	47.403	-2.426	1.00 80.73	8
ATOM	243	N	ASP	851	-1.168	45.352	-2.147	1.00 74.44	7
ATOM	244	CA	ASP	851	-0.137	45.775	-1.223	1.00 74.44	6
ATOM	245	CB	ASP	851	-0.163	44.913	0.034	1.00100.00	6
ATOM	245	CG	ASP	851	-0.724	45.642	1.229	1.00100.00	6
	247		ASP	851	-1.307	46.731	1.026	1.00100.00	8
ATOM	247		ASP	851	-0.588	45.124	2.360	1.00100.00	8
ATOM				851	1.159	45.518	-1.967	1.00 74.44	6
ATOM	249	C	ASP		1.583	44.367	-2.118	1.00 74.44	8
ATOM	250	0	ASP	851		46.581	-2.456	1.00 26.66	7
MOTA	251	N	ALA	852	1.775		-3.173	1.00 26.66	6
ATOM	252	CA	ALA	852	3.023	46.431	-4.475	1.00 20.00	6
ATOM	253	CB	ALA	852	2.984	47.212		1.00 26.66	6
ATOM	254	C	ALA	852	4.155	46.921	-2.313		8
ATOM	255	0	ALA	852	3.957	47.275	-1.154	1.00 26.66	7
ATOM	256	N	ALA	853	5.346	46.931	-2.890	1.00 89.52	
ATOM	257	CA	ALA	853	6.532	47.410	-2.204	1.00 89.52	6
MOTA	258	CB	ALA	853	7.355	46.243	-1.675	1.00 23.28	6
MOTA	259	C	ALA	853	7.324	48.210	-3.229	1.00 89.52	6
ATOM	260	0	ALA	853	7.765	47.668	-4.240	1.00 89.52	8
ATOM	261	N	ILE	854	7.417	49.467	-3.319	1.00 41.73	7
ATOM	262	CA	ILE	854	8.279	50.444	-3.999	1.00 41.73	6
ATOM	263	CB	ILE	854	7.851	51.866	-3.630	1.00 71.42	6
ATOM	264	CG2	ILE	854	8.539	52.937	-4.479	1.00 83.27	6
ATOM	265	CG1	ILE	854	6.349	52.102	-3.802	1.00 83.27	6
ATOM	266	CD1	ILE	854	5.768	51.388	-5.024	1.00 83.27	6
ATOM	267	С	ILE	854	9.736	50.239	-3.577	1.00 41.73	6
ATOM	268	ō	ILE	854	10.035	50.042	-2.390	1.00 41.73	8
ATOM	269	N	LYS	855	10.597	50.294	-4.576	1.00 62.34	7
ATOM	270	CA	LYS	855	12.045	50.123	-4.395	1.00 62.34	6
ATOM	271	CB	LYS	855	12.496	48.792	-5.001	1.00 99.81	6
ATOM	272	CG	LYS	855	13.652	48.147	-4.235	1.00 99.81	6
ATOM	273	CD	LYS	855	13.741	46.635	-4.449	1.00 99.81	6
ATOM	274	CE	LYS	855	13.407	46.212	-5.881	1.00 99.81	6
ATOM	275	NZ	LYS	855	14.507	46.460	-6.824	1.00 99.81	7
ATOM	2/5	14.25	пто	دده	14.307	30.400	0.024		

MOTA	276	С	LYS	855	12.797	51.263	-5.085	1.00 62.34	6
ATOM	277	0	LYS	855	12.216	52.028	-5.869	1.00 62.34	8
ATOM	278	N	ARG	856	14.076	51.334	-4.765	1.00100.00	7
ATOM	279	CA	ARG	856	14.982	52.353	-5.313	1.00100.00	6
ATOM	280	CB	ARG	856	14.324	53.733	-5.241	1.00 95.22	6
ATOM	281	CG	ARG	856	15.161	54.829	-5.903	1.00 95.22	6
ATOM	282	CD	ARG	856	14.465	56.192	-5.906	1.00 95.22	6
ATOM	283	NE	ARG	856	15.316	57.271	-6.428	1.00 95.22	7
ATOM	284	CZ	ARG	856	14.938	58.554	-6.503	1.00 95.22	6
ATOM	285	NH1		856	13.723	58.940	-6.093	1.00 95.22	7
ATOM	286	NH2		856	15.715	59.537	-6.979	1.00 95.22	7
ATOM	287	C	ARG	856	16.284	52.382	-4.510	1.00100.00	6
ATOM	288	0	ARG	856	16.269	52.404	-3.270	1.00100.00	8
ATOM	289	N	MET	857	17.443	52.378	-5.338	1.00100.00	7
ATOM	290	CA	MET	857	18.288	53.750	-3.743	1.00100.00	6
ATOM	291	CB	MET	857	18.449	53.730	-2.384	1.00100.00	6
ATOM	292	CG	MET	857	17.994	54.017	-1.306	1.00100.00	6
ATOM	292	SD	MET	857	18.352	53.350	0.258	1.00100.00	16
							0.204	1.00100.00	6
ATOM	294	CE	MET	857	20.116	53.447		1.00100.00	6
MOTA	295	C	MET	857	19.646	53.843	-4.450		8
ATOM	296	0	MET	857	20.497	52.937	-4.253	1.00100.00	
ATOM TER	297	OXT	MET	857	19.839	54.838	-5.196	1.00 82.10	8
ATOM	298	CB	ASP	864	22.499	50 075	-11.088	1.00 55.87	6
ATOM	299	C	ASP	864	23.323		-12.792	1.00100.00	6
ATOM	300	0	ASP	864	22.981		-13.940	1.00100.00	8
ATOM	301	N	ASP	864	22.263		-10.688	1.00100.00	7
ATOM	301	CA	ASP	864	22.263		-11.734	1.00100.00	6
		N					-12.412	1.00100.00	7
ATOM	303	CA	ASP	865 865	24.599 25.670		-13.347	1.00100.00	6
ATOM	304							1.00100.00	6
ATOM	305	CB	ASP	865	26.925		-13.098		6
MOTA	306	C	ASP	865	25.951		-13.073	1.00100.00	8
ATOM	307	0	ASP	865	26.537		-13.902		7
MOTA	308	N	HIS	866	25.485		-11.889	1.00 99.63	
MOTA	309	CA	HIS	866	25.554		-11.357	1.00 99.63	6
ATOM	310	CB	HIS	866	25.728	54.726	-9.827	1.00100.00	6
ATOM	311	CG	HIS	866	24.600	55.378	-9.079	1.00100.00	6
ATOM	312		HIS	866	23.472	54.858	-8.543	1.00100.00	6
ATOM	313		HIS	866	24.593	56.720	-8.769	1.00100.00	7
ATOM	314		HIS	866	23.509	57.002	-8.065	1.00100.00	6
ATOM	315		HIS	866	22.811	55.888	-7.915	1.00100.00	7
ATOM		- C	HIS	866	24.196		-11.715	1.00 99.63	6
MOTA	317	0	HIS	866	23.599		-10.964	1.00 99.63	8
ATOM	318	N	ARG	867	23.732		-12.904	1.00100.00	7
ATOM	319	CA	ARG	867	22.419		-13.405	1.00100.00	6
MOTA	320	CB	ARG	867	21.700		-13.954	1.00100.00	6
ATOM	321	CG	ARG	867	21.971	55.721	-15.445	1.00100.00	6
ATOM	322	CD	ARG	867	23.460	55.680	-15.790	1.00100.00	6
ATOM	323	NE	ARG	867	23.698	55.859	-17.219	1.00100.00	7
ATOM	324	CZ	ARG	867	24.794	55.439	-17.837	1.00100.00	6
ATOM	325	NH1	ARG	867	25.733	54.810	-17.137	1.00100.00	7
ATOM	326	NH2	ARG	867	24.940	55.628	-19.145	1.00100.00	7
ATOM	327	C	ARG	867	22.524	53.015	-14.480	1.00100.00	6
ATOM	328	0	ARG	867	21.980	53.140	-15.575	1.00100.00	8
ATOM	329	N	ASP	868	23.225	51.934	-14.164	1.00100.00	7
ATOM	330	CA	ASP	868	23.393		-15.146	1.00100.00	6
ATOM	331	CB	ASP	868	24.591		-14.773	1.00100.00	6

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Inventors:

MOTA 332 CG ASP 868 24.412 49.314 -13.435 1.00100.00 ATOM 333 OD1 ASP 868 24.613 49.980 -12.391 1.00100.00 ATOM 334 OD2 ASP 868 24.027 48.130 -13.442 1.00100.00 ATOM 335 C ASP 868 22.154 49.960 -15.282 1.00100.00 ATOM 336 O ASP 868 22.293 48.750 -15.504 1.00100.00 337 N PHE 869 ATOM 20.955 50.538 -15.156 1.00100.00 ATOM 338 CA PHE 869 19.717 49.746 -15.259 1.00100.00 ATOM 339 CB PHE 869 18.424 50.554 -15.017 1.00 99.62 18.424 50.554 -15.017 1.00 99.62 18.595 52.044 -14.986 1.00 99.62 18.716 52.692 -13.761 1.00 99.62 18.498 52.813 -16.148 1.00 99.62 18.734 54.068 -13.681 1.00 99.62 18.515 54.204 -16.077 1.00 99.62 ATOM 340 CG PHE 869 ATOM 341 CD1 PHE 869 ATOM 869 342 CD2 PHE ATOM 343 CE1 PHE 869 MOTA 344 CE2 PHE 869 MOTA 345 CZ PHE 869 18.630 54.834 -14.843 1.00 99.62 346 C ATOM PHE 869 19.576 49.080 -16.612 1.00100.00 PHE 869 ATOM 347 0 20.380 49.305 -17.508 1.00100.00 ATOM 348 N ALA 870 18.524 48.278 -16.746 1.00100.00 ATOM 349 CA ALA 870 18.206 47.512 -17.951 1.00100.00 ATOM 350 CB ALA 870 19.005 48.006 -19.156 1.00 97.10 ATOM 351 C ALA 870 18.532 46.061 -17.670 1.00100.00 MOTA 352 O ALA 870 17.644 45.222 -17.671 1.00100.00 ATOM 353 N GLY 871 19.810 45.775 -17.434 1.00100.00 ATOM 354 CA GLY 871 20.221 44.419 -17.133 1.00100.00 ATOM 355 C GLY 871 19.602 44.044 -15.804 1.00100.00 ATOM 356 0 GLY 871 19.400 42.871 -15.506 1.00100.00 ATOM 357 N GLU 872 19.305 45.055 -14.996 1.00 99.97 19.305 45.055 -14.996 1.00 99.97 18.669 44.813 -13.718 1.00 99.97 18.811 46.023 -12.787 1.00100.00 17.496 46.495 -12.182 1.00100.00 17.571 46.692 -10.675 1.00100.00 18.323 47.585 -10.230 1.00100.00 16.882 45.946 -9.940 1.00100.00 17.200 44.565 -14.033 1.00 99.97 ATOM 358 CA GLU 872 359 CB GLU 872 ATOM ATOM 360 CG GLU 872 361 CD GLU 872 ATOM 362 OE1 GLU 872 363 OE2 GLU 872 364 C GLU 872 365 O GLU 872 365 N LEU 873 367 CA LEU 873 ATOM ATOM ATOM 17.200 44.565 -14.033 1.00 99.97 ATOM 16.575 43.673 -13.465 1.00 99.97 ATOM 16.659 45.350 -14.961 1.00 63.02 ATOM 15.255 45.213 -15.327 1.00 63.02 ATOM 368 CB LEU 873 14.756 46.482 -15.955 1.00 69.97 ATOM 369 C LEU 873 14.977 44.032 -16.243 1.00 63.02 ATOM 370 0 LEU 873 13.990 43.323 -16.052 1.00 63.02 ATOM 371 N GLU 874 15.847 43.819 -17.227 1.00100.00 ATOM 372 CA GLU 874 15.687 42.716 -18.164 1.00100.00 ATOM 373 CB GLU 874 16.645 42.862 -19.331 1.00 19.50 MOTA 374 C GLU 874 15.923 41.394 -17.454 1.00100.00 ATOM 375 O GLU 874 15.103 40.482 -17.547 1.00100.00 376 N VAL 875 ATOM 17.040 41.298 -16.737 1.00 69.27 377 CA VAL 875 ATOM 17.383 40.082 -16.002 1.00 69.27 378 CB VAL 875 ATOM 18.763 40.218 -15.359 1.00 39.27 VAL 875 ATOM 379 C 16.344 39.755 -14.934 1.00 69.27 380 0 VAL 875 ATOM 16.338 38.651 -14.399 1.00 69.27 LEU 876 381 N ATOM 15.493 40.728 -14.613 1.00 78.00 382 CA LEU 876 ATOM 14.438 40.543 -13.616 1.00 78.00 383 CB LEU 876 ATOM 14.169 41.853 -12.843 1.00 53.20 MOTA 384 CG LEU 876 14.939 42.141 -11.537 1.00 29.26 ATOM 385 CD1 LEU 876 14.466 43.420 -10.852 1.00 29.26 ATOM 386 CD2 LEU 876 14.715 40.969 -10.608 1.00 29.26 ATOM 387 C LEU 876 13.147 40.076 -14.290 1.00 78.00

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12.410 39.262 -13.737 1.00 78.00

 $\begin{array}{lll} \mbox{Docket/App No.:} & 2079.1037-001 \\ \mbox{Title: Method of Identifying Inhibitors of TIE-2} \\ \mbox{Inventors:} & \mbox{Nancy J. Bump $\it{et al.}$} \end{array}$

ATOM	389	N	CYS	877	12.870	40.591	-15.486	1.00 60.18	7
ATOM	390	CA	CYS	877	11.652		-16.191	1.00 60.18	6
ATOM	391	CB	CYS	877	11.199	41.317	-17.164	1.00100.00	6
ATOM	392	SG	CYS	877	12.370		-18.447	1.00100.00	16
ATOM	393	С	CYS	877	11.857		-16.916	1.00 60.18	6
ATOM	394	ō	CYS	877	11.194		-17.909	1.00 60.18	8
ATOM	395	N	LYS	878	12.788	38.094	-16.398	1.00 65.17	7
ATOM	396	CA	LYS	878	13.088		-16.964	1.00 65.17	6
ATOM	397	CB	LYS	878	14.593		-17.078	1.00 89.20	6
ATOM	398	CG	LYS	878	15.190		-18.092	1.00 52.09	6
ATOM	399	CD	LYS	878	16.693	37.453	-18.128	1.00 52.09	6
ATOM	400	CE	LYS	878	17.289	38.360	-19.216	1.00 52.09	6
ATOM	401	NZ	LYS	878	16.965	37.922	-20.614	1.00 52.09	7
ATOM	402	С	LYS	878	12.473	35.703	-16.091	1.00 65.17	6
ATOM	403	ō	LYS	878	12.100		-16.572	1.00 65.17	8
ATOM	404	N	LEU	879	12.365	35.982	-14.801	1.00100.00	7
ATOM	405	CA	LEU	879	11.752	35.044	-13.879	1.00100.00	6
ATOM	406	CB	LEU	879	12.480	35.052	-12.526	1.00 45.22	6
ATOM	407	CG	LEU	879	12.801		-11.904	1.00 46.30	6
ATOM	408		LEU	879	13.226	36.250	-10.462	1.00 46.30	6
ATOM	409		LEU	879	13.892		-12.704	1.00 46.30	6
ATOM	410	C	LEU	879	10.301	35.492	-13.717	1.00100.00	6
ATOM	411	ō	LEU	879	10.019	36.656	-13.405	1.00100.00	8
ATOM	412	N	GLY	880	9.381		-13.972	1.00 96.05	7
ATOM	413	CA	GLY	880	7.980	34.903	-13.848	1.00 96.05	6
ATOM	414	C	GLY	880	7.540		-12.409	1.00 96.05	6
ATOM	415	ō	GLY	880	8.358		-11.483	1.00 96.05	8
ATOM	416	N	HIS	881	6.236		-12.216	1.00 70.51	7
ATOM	417	CA	HIS	881	5.693		-10.876	1.00 70.51	6
ATOM	418	CB	HIS	881	4.178		-10.843	1.00 99.80	6
ATOM	419	CG	HIS	881	3.498	34.160	-9.629	1.00 99.80	6
ATOM	420		HIS	881	3.000	32.924	-9.383	1.00 99.80	6
ATOM	421	NDI	HIS	881	3.264	34.897	-8.484	1.00 99.80	7
ATOM	422		HIS	881	2.648	34.142	-7.592	1.00 99.80	6
ATOM	423	NE2	HIS	881	2.477	32.939	-8.110	1.00 99.80	7
ATOM	424	С	HIS	881	5.952	33.094	-10.384	1.00 70.51	6
ATOM	425	0	HIS	881	5.908	32.134	-11.147	1.00 70.51	8
ATOM	426	N	HIS	882	6.231	32.982	-9.104	1.00 45.83	7
ATOM	427	CA	HIS	882	6.404	31.672	-8.546	1.00 45.83	6
ATOM	428	CB	HIS	882	7.866	31.289	-8.449	1.00 14.81	6
ATOM	429.	CG	HIS	882	8.076	29.813	-8.295	1.00 29.81	6
ATOM	430	CD2	HIS	882	7.783	28.782	-9.126	1.00 29.81	6
ATOM	431	ND1	HIS	882	8.608	29.244	-7.167	1.00 29.81	7
ATOM	432		HIS	882	8.638	27.932	-7.299	1.00 29.81	6
ATOM	433	NE2	HIS	882	8.142	27.626	-8.484	1.00 29.81	7
ATOM	434	C	HIS	882	5.773	31.719	-7.182	1.00 45.83	6
ATOM	435	0	HIS	882	5.987	32.655	-6.411	1.00 45.83	8
ATOM	436	N	PRO	883	4.959	30.711	-6.873	1.00 37.21	7
ATOM	437	CD	PRO	883	4.747	29.405	-7.508	1.00 52.55	6
ATOM	438	CA	PRO	883	4.353	30.762	-5.556	1.00 37.21	6
ATOM	439	CB	PRO	883	3.821	29.336	-5.373	1.00 47.02	6
ATOM	440	CG	PRO	883	4.591	28.493	-6.316	1.00 52.55	6
ATOM	441	C	PRO	883	5.359	31.209	-4.487	1.00 37.21	6
ATOM	442	o	PRO	883	4.990	31.958	-3.579	1.00 37.21	8
ATOM	443	N	ASN	884	6.628	30.800	-4.601	1.00 24.86	7
ATOM	444	CA	ASN	884	7.619	31.198	-3.582	1.00 24.86	6
ATOM	445	CB	ASN	884	8.077	29.996	-2.714	1.00 18.47	6

Title: Method of Identifying Inhibitors of TIE-2 Inventors: Nancy J. Bump et al.

	ATOM	446	CG	ASN	884	7.553	28.671	-3.203	1.00 3	3.47	6
	ATOM	447	OD1	ASN	884	7.951	28.205	-4.243	1.00 3	3.47	8
	ATOM	448	ND2	ASN	884	6.674	28.052	-2.443	1.00 3	3.47	7
	ATOM	449	С	ASN	884	8.860	31.986	-4.022	1.00 2	4.86	6
	ATOM	450	0	ASN	884	9.996	31.540	-3.862	1.00 2		8
	ATOM	451	N	ILE	885	8.603	33.191	-4.518	1.00 4		7
	ATOM	452	CA	ILE	885	9.616	34.125	-4.986	1.00 4		6
	ATOM	453	CB	ILE	885	10.063	33.811	-6.435	1.00 2		6
	ATOM	454	CG2	ILE	885	10.616	35.056	-7.119	1.00 2		6
	ATOM	455	CG1	ILE	885	11.101	32.696	-6.451	1.00 2		6
	ATOM	456	CD1	ILE	885	11.855	32.614	-7.727	1.00 2		6
	ATOM	457	C	ILE	885	8.924	35.476	-5.013	1.00 4		6
	ATOM	458	0	ILE	885	7.845	35.596	-5.601	1.00 4		8
	ATOM	459	N	ILE	886	9.501	36.488	-4.373	1.00 3		7
	ATOM	460	CA	ILE	886	8.857	37.785	-4.434	1.00 3		6
	ATOM	461	CB	ILE	886	9.462	38.768	-3.414	1.00 1		6
	ATOM	462		ILE	886	9.259	40.221	-3.846	1.00 2		6
	ATOM	463		ILE	886	8.764	38.531	-2.075	1.00 2		6
	ATOM	464		ILE	886	9.230	39.402	-1.000	1.00 2		6
477	ATOM	465	C	ILE	886	8.969	38.250	-5.881	1.00 2		6
60	ATOM	466	0	ILE	886	10.040	38.615	-6.363	1.00 3		8
13	ATOM	467	N	ASN	887	7.832	38.163	-6.566		9.60	7
(0	ATOM	468	CA	ASN	887	7.716	38.506	-7.975		9.60	6
- Septe	ATOM	469	CB	ASN	887	6.531	37.759	-8.603	1.00 8		6
Un	ATOM	470	CG	ASN	887	6.602	36.250	-8.406	1.00 8		6
W	ATOM	471		ASN	887	7.490				2.94	8
160	ATOM	472		ASN	887		35.584	-8.932	1.00 8		7
jede .						5.665	35.710	-7.637			
	ATOM	473	C	ASN	887	7.535	39.990	-8.222	1.00 3		6
i di	ATOM	474	0	ASN LEU	887	6.893	40.687	-7.432	1.00 3		8
(m)	ATOM	475	N		888	8.125	40.438	-9.332	1.00 7		
14	ATOM	476	CA	LEU	888	8.067	41.822	-9.789		3.28	6
fu	ATOM	477	CB	LEU	888	9.044		-10.953	1.00 3		6
14	ATOM	478	CG	LEU	888	9.064		-11.721	1.00 1		6
(2)	ATOM	479		LEU	888	9.760		-10.873		8.51	6
finh	ATOM	480		LEU	888	9.809		-13.035	1.00 1		6
1	ATOM	481	C	LEU	888	6.651		-10.274		3.28	6
	ATOM	482	0	LEU	888	6.083		-11.022	1.00 7		8
	ATOM	483	N	LEU	889	6.091	43.210	-9.853	1.00 9		7
	ATOM	484	CA	LEU	889	4.731		-10.235	1.00 9		6
	ATOM	485	CB	LEU	889	3.936	43.972	-8.975	1.00 9		6
	ATOM	486	CG	LEU	889	3.874	42.924	-7.838	1.00 5		6
	ATOM	487		LEU	889	2.923	43.357	-6.733	1.00 5		6
	ATOM	488		LEU	889	3.419	41.589	-8.413	1.00 5		6
	ATOM	489	C	LEU	889	4.676		-11.304	1.00 9	9.59	6
	ATOM	490	0	LEU	889	3.805	44.645	-12.167	1.00 9	9.59	8
	ATOM	491	N	GLY	890	5.599	45.636	-11.266	1.00 5	4.35	7
	ATOM	492	CA	GLY	890	5.597	46.699	-12.264	1.00 5	4.35	6
	ATOM	493	C	GLY	890	6.668	47.737	-11.986	1.00 5	4.35	6
	ATOM	494	0	GLY	890	7.617	47.466	-11.259	1.00 5	4.35	8
	ATOM	495	N	ALA	891	6.534	48.926	-12.560	1.00 6	6.65	7
	ATOM	496	CA	ALA	891	7.515	49.985	-12.328	1.00 6	6.65	6
	ATOM	497	CB	ALA	891	8.872	49.590	-12.911	1.00 6	8.11	6
	ATOM	498	C	ALA	891	7.055	51.299	-12.937	1.00 6	6.65	6
	ATOM	499	0	ALA	891	6.176	51.318	-13.789	1.00 6	6.65	8
	ATOM	500	N	CYS	892	7.656		-12.485	1.00 9	9.57	7
	ATOM	501	CA	CYS	892	7.322		-12.984	1.00 9	9.57	6
	MOTA	502	CB	CYS	892	6.872	54.619	-11.833	1.00 9	8.88	6

ATOM	503	SG	CYS	892	5.614	55 000	-12.345	1.00 92.24	16
ATOM		C	CYS	892	8.579	54.284	-12.345	1.00 92.24	10
ATOM		0	CYS	892	9.610	53.625	-13.611	1.00 99.57	8
ATOM	505	N	GLU	893	8.503	55.485	-14.165	1.00 99.69	7
ATOM		CA	GLU	893 893	9.676	56.130	-14.165	1.00 99.69	6
							-14.759	1.00100.00	6
ATOM	508 509	CB	GLU	893 893	9.687 10.439	55.991 54.776	-16.825	1.00100.00	6
			GLU					1.00100.00	6
ATOM	510	CD		893	10.793	54.883	-18.308		8
ATOM		OE1		893	11.715	55.657	-18.646	1.00100.00	8
ATOM	512		GLU	893	10.123	54.219	-19.128		
ATOM	513	C	GLU	893	9.616	57.594	-14.387	1.00 99.69	6 8
ATOM	514	0	GLU	893	9.817		-15.215		7
ATOM		N	HIS	894	9.516	57.779	-12.908	1.00 96.96	
ATOM	516	CA	HIS	894	9.344		-12.428	1.00 96.96	6
ATOM	517	CB	HIS	894	8.697	59.154	-11.042	1.00100.00	6
ATOM	518	CG	HIS	894	8.186		-10.618	1.00100.00	6
ATOM	519		HIS	894	7.291	61.381	-11.187	1.00100.00	6
ATOM	520		HIS	894	8.631	61.157	-9.457	1.00100.00	7
ATOM	521		HIS	894	8.019	62.323	-9.357	1.00100.00	6
ATOM	522	NE2	HIS	894	7.216		-10.381	1.00100.00	7
ATOM		C	HIS	894	10.703	59.854	-12.336	1.00 96.96	6
ATOM		0	HIS	894	11.756		-12.319	1.00 96.96	8
ATOM		N	ARG	895	10.631	61.171	-12.278	1.00100.00	7
ATOM		CA	ARG	895	11.818	62.033	-12.182	1.00100.00	6
ATOM		CB	ARG	895	11.408		-11.741	1.00100.00	6
ATOM		CG	ARG	895	10.703		-12.846	1.00100.00	6
ATOM		CD	ARG	895	10.357	65.661	-12.430	1.00100.00	6
ATOM		NE	ARG	895	10.896	66.673	-13.350	1.00100.00	7
ATOM		CZ	ARG	895	10.138	67.483	-14.101	1.00100.00	6
ATOM		NH1		895	8.801		-14.056	1.00100.00	7
ATOM		NH2	ARG	895	10.630	68.406	-14.939	1.00100.00	7
ATOM		C	ARG	895	12.796	61.452	-11.159	1.00100.00	6
ATOM		0	ARG	895	12.399	60.726	-10.236	1.00100.00	8
ATOM		N	GLY	896	14.055	61.795	-11.359	1.00100.00	7
ATOM		CA	GLY	896	15.150	61.337	-10.493	1.00100.00	6
ATOM		С	GLY	896	14.949	59.861	-10.145	1.00100.00	6
ATOM		0	GLY	896	14.575	59.517	-9.013	1.00100.00	8
ATOM		N	TYR	897	15.205	59.037	-11.143	1.00100.00	7
ATOM		CA	TYR	897	15.068	57.578	-11.033	1.00100.00	6
MOTA		CB	TYR	897	15.624	57.096	-9.692	1.00100.00	6
ATOM	543	CG	TYR	897	15.964	55.604	-9.688	1.00100.00	6
MOTA			TYR	897	17.195	55.165	-10.192	1.00100.00	6
ATOM	545	CE1	TYR	897	17.506	53.800	-10.190	1.00100.00	6
ATOM	546	CD2	TYR	897	15.045	54.676	-9.182	1.00100.00	6
ATOM	547	CE2	TYR	897	15.357	53.311	-9.179	1.00100.00	6
ATOM	548	CZ	TYR	897	16.587	52.873	-9.684	1.00100.00	6
ATOM	549	OH	TYR	897	16.890	51.547	-9.682	1.00100.00	8
ATOM	550	C	TYR	897	13.592	57.190	-11.131	1.00100.00	6
ATOM	551	0	TYR	897	12.714	58.051	-11.293	1.00100.00	8
ATOM	552	N	LEU	898	13.367	55.894	-11.027	1.00100.00	7
ATOM	553	CA	LEU	898	12.020	55.310	-11.093	1.00100.00	6
ATOM		CB	LEU	898	11.960	54.258	-12.202	1.00 41.85	6
ATOM		C	LEU	898	11.672	54.648	-9.759	1.00100.00	6
ATOM	556	0	LEU	898	12.234	54.992	-8.709	1.00100.00	8
ATOM		N	TYR	899	10.747	53.711	-9.850	1.00 72.77	7
ATOM		CA	TYR	899	10.267	52.951	-8.688	1.00 72.77	6
ATOM		CB	TYR	899	9.153	53.725	-7.982	1.00100.00	6

ATOM	560	CG	TYR	899	9.685	54.728	-6.958	1.00100.00	6
ATOM	561	CD1	TYR	899	9.394	56.090	-7.096	1.00100.00	6
ATOM	562	CE1	TYR	899	9.884	57.008	-6.159	1.00100.00	6
ATOM	563	CD2	TYR	899	10.465	54.283	-5.884	1.00100.00	6
ATOM	564	CE2	TYR	899	10.955	55.201	-4.948	1.00100.00	6
ATOM	565	CZ	TYR	899	10.664	56.564	-5.085	1.00100.00	6
ATOM	566	OH	TYR	899	11.140	57.456	-4.175	1.00100.00	8
ATOM	567	C	TYR	899	9.726	51.592	-9.136	1.00100.00	6
ATOM	568	ō	TYR	899	8.785	51.513	-9.940	1.00 72.77	8
ATOM	569	N	LEU	900	10.350	50.565	-8.591	1.00 72.77	7
ATOM	570	CA	LEU	900	9.996	49.168	-8.876	1.00 78.27	6
ATOM	571	CB	LEU	900	11.233	48.277	-8.738	1.00 78.27	6
ATOM	572	CG	LEU	900	11.566	47.512	-10.020	1.00 54.43	6
ATOM	573	CD1	LEU	900	11.602	48.408	-11.259	1.00 54.43	6
ATOM	574	CD2	LEU	900	12.931	46.823	-9.967	1.00 54.43	6
ATOM	575	CD2	LEU	900	8.927			1.00 54.43	6
ATOM	576	ō	LEU	900	9.079	48.689	-7.892 -6.669	1.00 78.27	8
ATOM ATOM	577	N	ALA	901	7.874	48.141	-8.468	1.00 78.27	7
ATOM	578	CA	ALA	901					
ATOM					6.731	47.614	-7.708	1.00 72.23	6
	579	CB	ALA	901	5.424	47.944	-8.433	1.00 33.79	6
ATOM	580	С	ALA	901	6.851	46.095	-7.568	1.00 72.23	6
ATOM	581	0	ALA	901	7.121	45.383	-8.546	1.00 72.23	8
ATOM	582	N	ILE	902	6.929	45.582	-6.293	1.00 59.87	7
ATOM	583	CA	ILE	902	7.104	44.154	-6.059	1.00 59.87	6
ATOM	584	CB	ILE	902	8.550	43.900	-5.623	1.00 34.80	6
ATOM	585	CG2	ILE	902	9.522	44.289	-6.729	1.00 35.77	6
ATOM	586	CG1	ILE	902	8.846	44.755	-4.397	1.00 35.77	6
ATOM	587	CD1	ILE	902	10.311	45.018	-4.169	1.00 35.77	6
ATOM	588	C	ILE	902	6.165	43.633	-4.969	1.00 59.87	6
ATOM	589	0	ILE	902	5.750	44.390	-4.093	1.00 59.87	8
ATOM	590	И	GLU	903	5.835	42.344	-5.030	1.00 34.73	7
ATOM	591	CA	GLU	903	4.967	41.716	-4.036	1.00 34.73	6
ATOM	592	CB	GLU	903	5.047	40.197	-4.119	1.00 38.01	6
ATOM	593	CG	GLU	903	4.180	39.568	-5.170	1.00 49.25	6
MOTA	594	CD	GLU	903	4.216	38.043	-5.112	1.00 49.25	6
ATOM	595		GLU	903	4.310	37.497	-3.985	1.00 49.25	8
ATOM	596	OE2	GLU	903	4.141	37.403	-6.191	1.00 49.25	8
ATOM	597	C	GLU	903	5.343	42.124	-2.627	1.00 34.73	6
MOTA	598	0	GLU	903	6.514	42.378	-2.330	1.00 34.73	8
MOTA	599	14	TYR	904	4.328	42.169	-1.770	1.00 31.03	7
ATOM	600	CA	TYR	904	4.469	42.530	-0.370	1.00 31.03	6
ATOM	601	CB	TYR	904	3.411	43.577	-0.003	1.00 13.64	6
ATOM	602	CG	TYR	904	3.419	43.950	1.459	1.00 23.21	6
ATOM	603	CD1	TYR	904	4.598	44.344	2.086	1.00 23.21	6
ATOM	604	CE1	TYR	904	4.647	44.606	3.448	1.00 23.21	6
ATOM	605	CD2	TYR	904	2.276	43.840	2.236	1.00 23.21	6
ATOM	606	CE2	TYR	904	2.315	44.102	3.608	1.00 23.21	6
ATOM	607	CZ	TYR	904	3.509	44.477	4.204	1.00 23.21	6
ATOM	608	OH	TYR	904	3.575	44.663	5.569	1.00 23.21	8
MOTA	609	C	TYR	904	4.328	41.291	0.532	1.00 31.03	6
ATOM	610	0	TYR	904	3.388	40.494	0.393	1.00 31.03	8
ATOM	611	N	ALA	905	5.284	41.154	1.447	1.00 31.20	7
ATOM	612	CA	ALA	905	5.334	40.063	2.409	1.00 31.20	6
ATOM	613	CB	ALA	905	6.733	39.460	2.430	1.00 28.71	6
ATOM	614	C	ALA	905	4.990	40.633	3.781	1.00 31.20	6
ATOM	615	0	ALA	905	5.853	41.091	4.514	1.00 31.20	8
ATOM	616	N	PRO	906	3.716	40.600	4.151	1.00 17.48	7

ATOM	617	CD	PRO	906	2.597	40.048	3.370	1.00 32.19	6
ATOM	618	CA	PRO	906	3.241	41.121	5.427	1.00 17.48	6
ATOM	619	CB	PRO	906	1.728	40.964	5.314	1.00 32.19	6
ATOM	620	CG	PRO	906	1.580	39.762	4.442	1.00 32.19	6
ATOM	621	С	PRO	906	3.774	40.564	6.724	1.00 17.48	6
ATOM	622	0	PRO	906	3.408	41.072	7.788	1.00 17.48	8
ATOM	623	N	HIS	907	4.636	39.550	6.683	1.00 30.66	7
ATOM	624	CA	HIS	907	5.123	38.987	7.954	1.00 30.66	6
MOTA	625	CB	HIS	907	4.657	37.543	8.130	1.00 5.00	6
ATOM	626	CG	HIS	907	3.174	37.357	8.048	1.00 5.00	6
ATOM	627	CD2	HIS	907	2.219	37.353	9.011	1.00 5.00	6
ATOM	628	ND1	HIS	907	2.517	37.103	6.865	1.00 5.00	7
ATOM	629	CE1	HIS	907	1.224	36.945	7.097	1.00 5.00	6
ATOM	630	NE2	HIS	907	1.021	37.091	8.393	1.00 5.00	7
ATOM	631	C	HIS	907	6.622	39.004	8.229	1.00 30.66	6
ATOM	632	0	HIS	907	7.130	38.115	8.926	1.00 30.66	8
ATOM	633	N	GLY	908	7.326	40.009	7.718	1.00 38.98	7
ATOM	634	CA	GLY	908	8.756	40.081	7.947	1.00 38.98	6
ATOM	635	С	GLY	908	9.483	38.924	7.298	1.00 38.98	6
ATOM	636	0	GLY	908	8.935	38.235	6.436	1.00 38.98	8
ATOM	637	N	ASN	909	10.719	38.698	7.718	1.00 31.42	7
ATOM	638	CA	ASN	909	11.517	37.620	7.140	1.00 31.42	6
ATOM	639	CB	ASN	909	12.963	38.068	6.941	1.00 41.70	6
ATOM	640	CG	ASN	909	13.566	38.630	8.197	1.00 41.70	6
ATOM	641		ASN	909	14.196	39.684	8.168	1.00 41.70	8
ATOM	642	ND2	ASN	909	13.381	37.931	9.316	1.00 41.70	7
ATOM	643	С	ASN	909	11.488	36.349	7.964	1.00 31.42	6
ATOM	644	0	ASN	909	11.094	36.340	9.132	1.00 31.42	8
ATOM	645	N	LEU	910	11.937	35.275	7.347	1.00 17.12	7
ATOM	646	CA	LEU	910	11.930	34.014	8.019	1.00 17.12	6
ATOM	647	CB	LEU	910	12.524	32.962	7.139	1.00 20.29	6
ATOM	648	CG	LEU	910	12.192	31.558	7.604	1.00 20.29	6
ATOM	649	CD1	LEU	910	10.687	31.274	7.677	1.00 20.29	6
ATOM .	650	CD2	LEU	910	12.850	30.696	6.590	1.00 20.29	6
ATOM	651	C	LEU	910	12.679	34.039	9.332	1.00 17.12	6
MOTA	652	0	LEU	910	12.183	33.554	10.355	1.00 17.12	8
ATOM	653	N	LEU	911	13.885	34.579	9.319	1.00 21.04	7
ATOM	654	CA	LEU	911	14.646	34.644	10.551	1.00 21.04	6
ATOM	655	CB	LEU	911	15.865	35.523	10.363	1.00 23.99	6
ATOM	656	CG	LEU	911	16.744	35.463	11.596	1.00 23.99	6
MOTA	657	CD1	LEU	911	17.326	34.053	11.797	1.00 23.99	6
MOTA	658	CD2	LEU	911	17.833	36.483	11.399	1.00 23.99	6
ATOM	659	C	LEU	911	13.791	35.199	11.697	1.00 21.04	6
ATOM	660	0	LEU	911	13.565	34.515	12.692	1.00 21.04	8
ATOM	661	N	ASP	912	13.305	36.429	11.557	1.00 16.81	7
ATOM	662	CA	ASP	912	12.489	37.041	12.618	1.00 16.81	6
ATOM	663	CB	ASP	912	11.973	38.399	12.177	1.00 39.39	6
MOTA	664	CG	ASP	912	12.996	39.463	12.327	1.00 39.39	6
ATOM	665	OD1	ASP	912	12.794	40.557	11.777	1.00 39.39	8
ATOM	666	OD2	ASP	912	14.005	39.185	12.989	1.00 39.39	8
MOTA	667	C	ASP	912	11.311	36.214	13.031	1.00 16.81	6
ATOM	668	0	ASP	912	11.020	36.079	14.215	1.00 16.81	8
MOTA	669	N	PHE	913	10.623	35.698	12.027	1.00 39.11	7
ATOM	670	CA	PHE	913	9.462	34.884	12.255	1.00 39.11	6
ATOM	671	CB	PHE	913	8.850	34.495	10.937	1.00 34.21	6
ATOM	672	CG	PHE	913	7.458	34.005	11.055	1.00 34.21	6
MOTA	673	CD1	PHE	913	6.412	34.897	11.233	1.00 34.21	6

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7.635 30.893 24.867 1.00 29.42 6

Inventors:

ATOM

787 N

ATOM 731 0 VAL 919 7.173 31.537 25.793 1.00 29.42 732 N LEU 920 ATOM 8.635 30.048 25.020 1.00 34.37 ATOM 733 CA LEU 920 9.260 29.900 26.305 1.00 34.37 ATOM 734 CB LEU 920 10.093 28.629 26.324 1.00 36.03 ATOM 735 CG LEU 920 10.688 28.310 27.688 1.00 36.03 ATOM 736 CD1 LEU 920 9.559 28.061 28.676 1.00 36.03 11.592 27.104 27.587 1.00 36.03 10.138 31.117 26.552 1.00 34.37 10.523 31.393 27.676 1.00 29.12 11.301 33.025 25.693 1.00 29.12 12.215 33.237 24.485 1.00 99.98 13.465 35.574 24.758 1.00 99.98 13.165 35.574 24.753 1.00 99.98 13.156 36.228 25.824 1.00 99.98 13.156 36.228 25.824 1.00 99.98 13.156 36.228 25.824 1.00 99.98 13.156 36.228 25.824 1.00 99.98 13.156 36.228 25.824 1.00 99.98 13.156 36.228 25.824 1.00 29.12 10.452 34.929 26.869 1.00 29.12 10.452 34.929 26.869 1.00 29.12 9.559 28.061 28.676 1.00 36.03 ATOM 737 CD2 LEU 920 738 C LEU 920 ATOM 920 ATOM 739 O LEU MOTA 740 N GLU 921 921 ATOM 741 CA GLU 742 CB GLU 921 743 CG GLU 921 744 CD GLU 921 745 OE1 GLU 921 ATOM ATOM ATOM ATOM 746 OE2 GLU 921 747 C GLU 921 748 O GLU 921 ATOM ATOM ATOM ATOM 749 N THR 922 9.455 34.375 24.932 1.00 52.74 ATOM 750 CA THR 922 8.463 35.437 24.944 1.00 52.74 ATOM 751 CB THR 922 7.450 35.207 23.800 1.00 53.34 ATOM 752 OG1 THR 922 8.038 35.598 22.558 1.00 53.34 ATOM 753 CG2 THR 922 6.167 35.977 24.026 1.00 53.34 ATOM 754 C THR 922 7.706 35.498 26.265 1.00 52.74 ATOM 755 O THR 922 7.923 36.398 27.077 1.00 52.74 ATOM 756 N ASP 923 6.827 34.515 26.461 1.00 32.25 5.981 34.391 27.651 1.00 32.25 ATOM 757 CA ASP 923 ATOM 758 CB ASP 923 4.509 34.434 27.231 1.00 60.93 3.558 34.328 28.404 1.00 60.93 ATOM 759 CG ASP 923 ATOM 760 OD1 ASP 923 3.762 35.032 29.415 1.00 60.93 761 OD2 ASP 923 [] ATOM 2.593 33.545 28.309 1.00 60.93 ATOM 762 C ASP 923 6.295 33.083 28.361 1.00 32.25 763 O ASP 923 764 N PRO 924 765 CD PRO 924 ATOM 5.711 32.034 28.055 1.00 32.25 ATOM 7.216 33.146 29.346 1.00 33.34 ATOM 7.426 34.381 30.130 1.00100.00 ATOM 766 CA PRO 924 7.637 31.978 30.125 1.00 33.34 ATOM 767 CB PRO 924 8.263 32.605 31.366 1.00100.00 ATOM 768 CG PRO 924 7.488 33.863 31.535 1.00100.00 ATOM PRO 924 769 C 6.464 31.030 30.456 1.00 33.34 ATOM 770 0 PRO 924 6.470 29.873 30.053 1.00 33.34 771 N ATOM ALA 925 5.460 31.543 31.164 1.00 69.10 ATOM 772 CA ALA 925 4.282 30.781 31.603 1.00 69.10 ATOM 773 CB ALA 925 3.311 31.735 32.255 1.00 73.73 ATOM 774 C ALA 925 3.562 29.976 30.531 1.00 69.10 3.562 29.976 30.531 1.00 69.10 3.802 28.779 30.384 1.00 69.10 2.662 30.639 29.806 1.00 48.64 1.877 30.013 28.743 1.00 48.64 1.766 30.975 27.558 1.00 37.88 0.669 30.632 26.605 1.00 37.88 ATOM 775 O ALA 925 ATOM 776 N PHE 926 777 CA PHE 926 ATOM 778 CB PHE 926 ATOM 779 CG PHE 926 ATOM 780 CD1 PHE 926 781 CD2 PHE 926 ATOM -0.646 30.983 26.893 1.00 37.88 ATOM 0.926 29.853 25.479 1.00 37.88 MOTA 782 CE1 PHE 926 -1.679 30.560 26.089 1.00 37.88 783 CE2 PHE 926 MOTA -0.106 29.420 24.668 1.00 37.88 MOTA 784 CZ PHE 926 -1.406 29.774 24.977 1.00 37.88 ATOM 785 C PHE 926 2.439 28.673 28.267 1.00 48.64 ATOM 786 O PHE 926 1.752 27.656 28.298 1.00 48.64

3.688 28.681 27.812 1.00 47.80 7

ALA 927

Nancy J. Bump et al Inventors:

	ATOM	788	CA	ALA	927	4.337	27.467	27.340	1.00 47.80	6
	ATOM	789	CB	ALA	927	5.786	27.752	26.970	1.00 31.97	6
	ATOM	790	C	ALA	927	4.272	26.297	28.314	1.00 47.80	6
	ATOM	791	0	ALA	927	3.725	25.256	27.984	1.00 47.80	8
	ATOM	792	N	ILE	928	4.850	26.439	29.499	1.00 44.35	7
	ATOM	793	CA	ILE	928	4.810	25.346	30.457	1.00 44.35	6
	ATOM	794	CB	ILE	928	5.155	25.837	31.868	1.00 67.81	6
	ATOM	795	CG2		928	5.834	24.735	32.641	1.00 29.96	6
	ATOM	796		ILE	928	6.130	27.004	31.806	1.00 29.96	6
	ATOM	797		ILE	928	7.542	26.594	31.485	1.00 29.96	6
	ATOM	798	C	ILE	928	3.410	24.718	30.494	1.00 44.35	6
	ATOM	799	ō	ILE	928	3.266	23.499	30.626	1.00 44.35	8
	ATOM	800	N	ALA	929	2.390	25.562	30.346	1.00 42.29	7
	ATOM	801	CA.	ALA	929	0.984	25.135	30.390	1.00 42.29	6
	ATOM	802	CB	ALA	929	0.118	26.315	30.330	1.00 42.29	6
	ATOM	803	C	ALA	929	0.457	24.440	29.156	1.00 42.29	6
	ATOM	804	0	ALA	929		23.429	29.252	1.00 42.29	8
						-0.225			1.00 42.29	7
	ATOM	805	N	ASN	930	0.745	24.995	27.994		
	ATOM	806	CA	ASN	930	0.259	24.398	26.775	1.00 36.17	6
	ATOM	807	CB	ASN	930	-0.230	25.506	25.852	1.00 57.20	6
(1)	MOTA	808	CG	ASN	930	-1.444	26.223	26.430	1.00 57.20	6
43	ATOM	809		ASN	930	-2.586	25.742	26.344	1.00 57.20	8
(0)	ATOM	810	ND2		930	-1.202	27.360	27.057	1.00 57.20	7
14	ATOM	811	C	ASN	930	1.295	23.486	26.128	1.00 36.17	6
	ATOM	812	0	ASN	930	1.088	22.976	25.028	1.00 36.17	8
M	ATOM	813	N	SER	931	2.401	23.259	26.834	1.00 50.28	7
1.12	ATOM	814	CA	SER	931	3.468	22.383	26.353	1.00 50.28	6
# m	ATOM	815	CB	SER	931	2.986	20.930	26.341	1.00 90.81	6
firet.	ATOM	816	OG	SER	931	2.790	20.433	27.659	1.00 90.81	8
8.	ATOM	817	C	SER	931	4.006	22.748	24.979	1.00 50.28	6
	ATOM	818	0	SER	931	4.484	21.889	24.258	1.00 50.28	8
W	ATOM	819	N	THR	932	3.918	24.023	24.622	1.00 48.32	7
ĨÜ	ATOM	820	CA	THR	932	4.397	24.510	23.334	1.00 48.32	6
	ATOM	821	CB	THR	932	3.443	25.591	22.749	1.00 79.61	6
FU.	ATOM	822		THR	932	3.247	26.634	23.711	1.00 79.61	8
63	ATOM	823	CG2	THR	932	2.108	24.989	22.374	1.00 79.61	6
frof.	ATOM	824	C	THR	932	5.784	25.127	23.483	1.00 48.32	6
	ATOM	825	0	THR	932	6.046	25.841	24.449	1.00 48.32	8
	ATOM	826	N	ALA	933	6.667	24.854	22.527	1.00 55.05	7
	ATOM	827	CA	ALA	933	8.009	25.436	22.552	1.00 55.05	6
	ATOM	828	CB	ALA	933	9.057	24.378	22.297	1.00 28.55	6
	ATOM	829	C	ALA	933	8.051	26.489	21.461	1.00 55.05	6
	ATOM	830	0	ALA	933	8.936	27.339	21.437	1.00 55.05	8
	ATOM	831	N	SER	934	7.098	26.393	20.543	1.00 27.13	7
	ATOM	832	CA	SER	934	6.978	27.340	19.469	1.00 27.13	6
	ATOM	833	CB	SER	934	7.937	27.003	18.341	1.00 36.98	6
	ATOM	834	OG	SER	934	7.630	27.748	17.167	1.00 36.98	8
	ATOM	835	C	SER	934	5.552	27.315	18.959	1.00 27.13	6
	ATOM	836	o	SER	934	4.897	26.270	19.001	1.00 27.13	8
	ATOM	837	N	THR	935	5.080	28.468	18.488	1.00 15.04	7
	ATOM	838	CA	THR	935	3.740	28.582	17.963	1.00 15.04	6
	ATOM	839	CB	THR	935	3.387	30.101	17.642	1.00 26.85	6
	ATOM	840	OG1		935	4.301	30.658	16.680	1.00 26.85	8
	ATOM	841	CG2	THR	935	3.432	30.930	18.917	1.00 26.85	6
	ATOM	842	C	THR	935	3.652	27.696	16.712	1.00 15.04	6
	ATOM	843	0	THR	935	2.594	27.154	16.407	1.00 15.04	8
	ATOM	844	N	LEU	936	4.778	27.530	16.015	1.00 41.56	7
						2	2230			-

ATOM	845	CA	LEU	936	4.839	26.720	14.788	1.00 41.56	6
ATOM	846	CB	LEU	936	6.005	27.210	13.915	1.00 16.11	6
ATOM	847	CG	LEU	936	5.980	28.713	13.613	1.00 16.11	6
ATOM	848	CD1		936	7.108	29.067	12.679	1.00 16.11	6
MOTA	849		LEU	936	4.640	29.083	13.020	1.00 16.11	6
ATOM	850	C	LEU	936	4.958	25.203	15.018	1.00 41.56	6
ATOM	851	0	LEU	936	5.433	24.744	16.063	1.00 41.56	8
MOTA	852	N	SER	937	4.524	24.440	14.021	1.00 27.35	7
ATOM	853	CA	SER	937	4.551	22.989	14.081	1.00 27.35	6
ATOM	854	CB	SER	937	3.167	22.438	13.764	1.00 9.94	6
ATOM	855	OG	SER	937	2.884	22.429	12.374	1.00 9.94	8
ATOM	856	C	SER	937	5.574	22.357	13.128	1.00 27.35	6
ATOM	857	0	SER	937	6.180	23.041	12.291	1.00 27.35	8
ATOM	858	N	SER	938	5.752	21.043	13.257	1.00 23.83	7
ATOM	859	CA	SER	938	6.689	20.294	12.431	1.00 23.83	6
ATOM	860	CB	SER	938	6.678	18.813	12.838	1.00 31.90	6
ATOM	861	OG	SER	938	7.011	17.966	11.741	1.00 31.90	8
ATOM	862	C	SER	938	6.362	20.431	10.943	1.00 23.83	6
ATOM	863	0	SER	938	7.256	20.590	10.121	1.00 23.83	8
ATOM	864	N	GLN	939	5.083	20.382	10.597	1.00 34.70	7
ATOM	865	CA	GLN	939	4.704	20.491	9.206	1.00 34.70	6
ATOM	866	CB	GLN	939	3.296	19.955	9.022	1.00 40.81	6
ATOM	867	CG	GLN	939	3.189	18.544	9.538	1.00 40.81	6
ATOM	868	CD	GLN	939	4.026	17.558	8.732	1.00 40.81	6
ATOM	869	0E1	GLN	939	3.584	17.084	7.675	1.00 40.81	8
ATOM	870	NE2	GLN	939	5.243	17.254	9.216	1.00 40.81	7
ATOM	871	С	GLN	939	4.838	21.906	8.685	1.00 34.70	6
ATOM	872	0	GLN	939	5.352	22.096	7.592	1.00 34.70	8
ATOM	873	N	GLN	940	4.388	22.906	9.435	1.00 22.70	7
ATOM	874	CA	GLN	940	4.556	24.267	8.950	1.00 22.70	6
ATOM	875	CB	GLN	940	4.094	25.286	9.986	1.00 30.92	6
ATOM	876	CG	GLN	940	4.588	26.679	9.679	1.00 30.92	6
ATOM	877	CD	GLN	940	3.663	27.483	8.790	1.00 30.92	6
ATOM	878	OE1	GLN	940	2.738	28.141	9.277	1.00 30.92	8
ATOM	879	NE2	GLN	940	3.891	27.427	7.482	1.00 30.92	7
ATOM	880	C	GLN	940	6.047	24.501	8.632	1.00 22.70	6
MOTA	881	0	GLN	940	6.381	25.050	7.574	1.00 22.70	8
ATOM	882	N	LEU	941	6.934	24.076	9.535	1.00 22.33	7
ATOM	883	CA	LEU	941	8.377	24.242	9.348	1.00 22.33	6
MOTA	884	CB	LEU	941	9.137	23.858	10.599	1.00 19.37	6
ATOM	885	CG	LEU	941	8.939	24.738	11.806	1.00 19.37	6
ATOM	886		LEU	941	9.540	23.981	12.995	1.00 19.37	6
ATOM	887	CD2	LEU	941	9.613	26.094	11.606	1.00 19.37	6
MOTA	888	C	LEU	941	8.956	23.427	8.202	1.00 22.33	6
ATOM	889	0	LEU	941	9.994	23.781	7.648	1.00 22.33	8
ATOM	890	N	LEU	942	8.334	22.308	7.869	1.00 30.49	7
ATOM	891	CA	LEU	942	8.877	21.545	6.765	1.00 30.49	6
MOTA	892	CB	LEU	942	8.370	20.098	6.748	1.00 27.17	6
ATOM	893	CG	LEU	942	8.901	19.138	7.816	1.00 27.17	6
ATOM	894	CD1		942	8.244	17.799	7.576	1.00 27.17	6
ATOM	895		LEU	942	10.399	18.997	7.776	1.00 27.17	6
ATOM	896	C	LEU	942	8.445	22.285	5.517	1.00 30.49	6
ATOM	897	0	LEU	942	9.211	22.408	4.582	1.00 30.49	8
ATOM	898	N	HIS	943	7.224	22.805	5.502	1.00 24.87	7
ATOM	899	CA	HIS	943	6.766	23.543	4.331	1.00 24.87	6
ATOM	900	CB	HIS	943	5.393	24.127	4.565	1.00 75.69	6
ATOM	901	CG	HIS	943	4.306	23.142	4.316	1.00 75.69	6

ATOM	902	ana	HIS	943	3.224	23.187	3.507	1.00 75.69	6
	902		HIS	943	4.317	21.892	4.884	1.00 75.69	7
ATOM			HIS	943	3.284	21.198	4.431	1.00 75.69	6
ATOM	904		HIS	943	2.608	21.960	3.596	1.00 75.69	7
ATOM	905			943	7.727	24.644	3.967	1.00 24.87	6
ATOM	906	C	HIS		8.112	24.794	2.815	1.00 24.87	8
ATOM	907	0	HIS	943	8.107	25.412	4.976	1.00 23.28	7
MOTA	908	N	PHE	944		26.499	4.812	1.00 23.28	6
MOTA	909	CA	PHE	944	9.049	27.069	6.196	1.00 24.44	6
ATOM	910	CB	PHE	944	9.379	27.059	6.782	1.00 24.44	6
ATOM	911	CG	PHE	944	8.293		8.101	1.00 24.44	6
ATOM	912	CD1	PHE	944	8.361	28.370		1.00 24.44	6
MOTA	913	CD2	PHE	944	7.282	28.477	5.983 8.598	1.00 24.44	6
MOTA	914	CE1	PHE	944	7.449	29.299			6
MOTA	915	CE2	PHE	944	6.372	29.406	6.489		6
MOTA	916	CZ	PHE	944	6.466	29.815	7.792	1.00 24.44	6
ATOM	917	C	PHE	944	10.301	26.011	4.079	1.00 23.28	
ATOM	918	0	PHE	944	10.778	26.675	3.164	1.00 23.28	8
ATOM	919	N	ALA	945	10.829	24.855	4.470	1.00 15.27	7
MOTA	920	CA	ALA	945	11.996	24.310	3.799	1.00 15.27	6
MOTA	921	CB	ALA	945	12.627	23.197	4.645	1.00 55.81	6
MOTA	922	С	ALA	945	11.644	23.804	2.386	1.00 15.27	6
MOTA	923	0	ALA	945	12.493	23.819	1.517	1.00 15.27	8
ATOM	924	N	ALA	946	10.408	23.368	2.139	1.00 9.68	7
ATOM	925	CA	ALA	946	10.011	22.897	0.795	1.00 9.68	6
ATOM	926	CB	ALA	946	8.734	22.042	0.869	1.00 20.69	6
ATOM	927	C	ALA	946	9.760	24.088	-0.114	1.00 9.68	6
MOTA	928	0	ALA	946	10.026	24.032	-1.319	1.00 9.68	8
ATOM	929	N	ASP	947	9.205	25.149	0.471	1.00 24.26	7
ATOM	930	CA	ASP	947	8.922	26.379	-0.245	1.00 24.26	6
ATOM	931	CB	ASP	947	8.300	27.430	0.671	1.00 51.33	6
ATOM	932	CG	ASP	947	6.870	27.122	1.021	1.00 51.33	6
ATOM	933	OD1	ASP	947	6.378	26.066	0.572	1.00 51.33	8
ATOM	934	OD2	ASP	947	6.248	27.934	1.740	1.00 51.33	8
ATOM	935	C	ASP	947	10.231	26.909	-0.772	1.00 24.26	6
ATOM	936	0	ASP	947	10.378	27.109	-1.979	1.00 24.26	8
ATOM	937	N	VAL	948	11.192	27.120	0.123	1.00 17.83	7
ATOM	938	CA	VAL	948	12.458	27.641	-0.335	1.00 17.83	6
ATOM	939	CB	VAL	948	13.483	27.833	0.788	1.00 5.04	6
ATOM	940	CG1	VAL	948	14.786	28.296	0.175	1.00 5.04	6
ATOM	941	CG2	VAL	948	13.012	28.856	1.801	1.00 5.04	6
ATOM	942	C	VAL	948	13.078	26.766	-1.412	1.00 17.83	6
ATOM	943	0	VAL	948	13.514	27.304	-2.425	1.00 17.83	8
ATOM	944	N	ALA	949	13.115	25.442	-1.219	1.00 24.98	7
ATOM	945	CA	ALA	949	13.697	24.531	-2.221	1.00 24.98	6
ATOM	946	CB	ALA	949	13.827	23.129	-1.666	1.00 53.47	6
ATOM	947	C	ALA	949	12.882	24.505	-3.505	1.00 24.98	6
ATOM	948	0	ALA	949	13.440	24.313	-4.576	1.00 24.98	8
ATOM	949	N	ARG	950	11.570	24.716	-3.413	1.00 23.96	7
ATOM	950	CA	ARG	950	10.742	24.733	-4.617	1.00 23.96	6
ATOM	951	СВ	ARG	950	9.239	24.736	-4.282	1.00 30.38	6
ATOM	952	CG	ARG	950	8.302	24.244	-5.419	1.00 30.38	6
ATOM	953	CD	ARG	950	6.829	24.454	-5.081	1.00 30.38	6
ATOM	954	NE	ARG	950	6.567	24.306	-3.648	1.00 30.38	7
ATOM	955	CZ	ARG	950	6.313	23.154	-3.030	1.00 30.38	6
ATOM	956		1 ARG	950	6.270		-3.723	1.00 30.38	7
ATOM	957	NH		950	6.132		-1.708	1.00 30.38	7
ATOM	958	C	ARG	950	11.091		-5.391		6
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ATOM

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LYS 958

Title: Method of Identifying Inhibitors of TIE-2 Nancy J. Bump et al.

ATOM 959 0 ARG 950 11.089 26.003 -6.617 1.00 23.96 ATOM 960 N GLY 951 11.409 27.064 -4.667 1.00 35.74 ATOM 961 CA GLY 951 11.749 28.315 -5.323 1.00 35.74 ATOM 962 C GLY 9.51 13.156 28.338 -5.890 1.00 35.74 ATOM 963 0 GLY 951 13.439 29.046 -6.850 1.00 35.74 14.050 27.562 -5.294 ATOM 964 N MET 952 1.00 35.49 ATOM 965 CA MET 952 15.430 27.512 -5.755 1.00 35.49 ATOM 966 CB MET 952 16.335 26.979 -4.656 1.00 28.83 ATOM 967 CG MET 952 16.616 27.981 -3.562 1.00 28.83 ATOM 968 SD MET 17.396 29.511 -4.180 1.00 28.83 952 ATOM 969 CE MET 18.963 28.883 952 -4.732 1.00 28.83 15.553 26.645 ATOM 970 C MET 952 -6.972 1.00 35.49 16.480 26.786 14.623 25.723 14.658 24.863 ATOM 971 0 MET 952 -7.759 1.00 35.49 ATOM 972 N ASP 953 -7.119 1.00 22.04 7 ATOM 973 CA ASP 953 -8,277 1.00 22.04 MOTA 974 CB ASP 953 13.701 23.708 -8.065 1.00 46.74 ATOM 975 CG ASP 953 13.868 22.649 -9.095 1.00 46.74 ATOM 976 OD1 ASP 953 14.938 22.016 -9.119 1.00 46.74 977 OD2 ASP ATOM 953 12.934 22.479 -9.894 1.00 46.74 ATOM 978 C ASP 953 14.285 25.650 -9.534 1.00 22.04 979 0 ATOM ASP 953 14.796 25.378 -10.600 1.00 22.04 ATOM 980 N TYR 954 13.388 26.620 -9.391 1.00 30.73 7 ATOM 981 CA TYR 954 12.969 27.454 -10.506 1.00 30.73 982 CB TYR 954 ATOM 11.735 28.261 -10.120 1.00 46.88 ATOM 983 CG TYR 954 11.212 29.222 -11.180 1.00 46.88 ATOM 984 CD1 TYR 954 10.358 28.777 -12.198 1.00 46.88 ATOM 985 CE1 TYR 954 9.817 29.675 -13.139 1.00 46.88 ATOM 986 CD2 TYR 954 11.523 30.596 -11.131 1.00 46.88 ATOM 987 CE2 TYR 954 10.987 31.498 -12.071 1.00 46.88 ATOM 988 CZ TYR 954 10.139 31.023 -13.062 1.00 46.88 ATOM 989 OH TYR 954 9.618 31.893 -13.980 1.00 46.88 ATOM TYR 954 990 C 14.104 28.406 -10.820 1.00 30.73 TYR 954 LEU 955 ATOM 991 0 14.484 28.556 -11.961 1.00 30.73 ATOM 992 N 14.654 29.048 -9.801 1.00 22.51 7 LEU 955 MOTA 993 CA 15.727 29.991 -10.043 1.00 22.51 MOTA 994 CB LEU 955 16.100 30.747 -8.771 1.00 36.85 ATOM 995 CG LEU 955 15.064 31.699 -8.184 1.00 36.85 ATOM 996 CD1 LEU 955 15.708 32.365 -7.021 1.00 36.85 ATOM 997 CD2 LEU 955 14.586 32.734 -9.210 1.00 36.85 ATOM 998 C LEU 955 16.963 29.355 -10.619 1.00 22.51 ATOM 999 0 LEU 955 17.530 29.885 -11.560 1.00 22.51 MOTA 1000 N SER 956 17.403 28.229 -10.080 1.00 31.05 ATOM 1001 CA SER 956 18.608 27.602 -10.615 1.00 31.05 ATOM 1002 CB SER 956 18.998 26.380 -9.778 1.00 57.17 ATOM 1003 OG SER 956 18.077 25.324 -9.989 1.00 57.17 ATOM 1004 C SER 956 18.439 27.207 -12.084 1.00 31.05 ATOM 1005 0 SER 956 19.379 27.348 -12.858 1.00 31.05 ATOM 1006 N GLN 957 17.247 26.732 -12.462 1.00 19.64 ATOM 1007 CA GLN 957 16.932 26.307 -13.841 1.00 19.64 ATOM 1008 CB GLN 957 1.00 97.55 15.580 25.587 -13.899 ATOM 1009 CG GLN 957 15.565 24.175 -13.366 1.00 97.55 ATOM 1010 CD GLN 957 16.884 23.460 -13.539 1.00 97.55 ATOM 1011 OE1 GLN 957 17.543 23.597 -14.568 1.00 97.55 ATOM 1012 NE2 GLN 957 17.275 22.679 -12.532 1.00 97.55 7 ATOM 1013 C GLN 957 16.901 27.437 -14.860 1.00 19.64 ATOM 1014 0 GLN 957 16.903 27.191 -16.054 1.00 19.64

16.815 28.666 -14.370 1.00 37.82

ATOM	1016	CA	LYS	958	16.801	29 851	-15.205	1.00 37.82	. 6
ATOM	1017	CB	LYS	958	15.881		-14.601	1.00 51.85	
ATOM	1018	CG	LYS	958	14.374		-14.569	1.00 51.85	
ATOM	1019	CD	LYS	958	13.831	30.551	-15.986	1.00 51.85	
ATOM	1020	CE	LYS	958	12.345		-16.083	1.00 51.85	
ATOM	1021	NZ	LYS	958	12.076		-17.526	1.00 51.85	
ATOM	1022	C	LYS	958	18.236				
ATOM	1023	0	LYS	958		30.355	-15.192	1.00 37.82	
ATOM	1023	N	GLN	959	18.528		-15.641	1.00 37.82	
ATOM	1024	CA	GLN		19.129		-14.634	1.00 37.14	
ATOM				959	20.543		-14.550	1.00 37.14	6
ATOM	1026 1027	CB	GLN	959	21.078		-15.942	1.00 59.23	6
		CG	GLN	959	20.943		-16.925	1.00 59.23	6
ATOM	1028	CD	GLN	959	21.605	27.827	-16.441	1.00 59.23	6
MOTA	1029		GLN	959	22.832	27.742	-16.372	1.00 59.23	8
ATOM	1030		GLN	959	20.790	26.844	-16.047	1.00 59.23	7
ATOM	1031	C	GLN	959	20.914	31.004	-13.559	1.00 37.14	6
ATOM	1032	0	GLN	959	21.937	31.669	-13.751	1.00 37.14	8
ATOM	1033	N	PHE	960	20.097	31.201	-12.519	1.00 48.69	7
ATOM	1034	CA	PHE	960	20.369	32.208	-11.492	1.00 48.69	6
ATOM	1035	CB	PHE	960	19.067	32.712	-10.840	1.00 18.22	6
ATOM	1036	CG	PHE	960	18.261	33.647	-11.686	1.00 18.22	6
MOTA	1037		PHE	960	17.426	33.166	-12.686	1.00 18.22	6
ATOM	1038		PHE	960	18.343	35.023	-11.493	1.00 18.22	6
MOTA	1039	CEl	PHE	960	16.677	34.044	-13.502	1.00 18.22	6
ATOM	1040	CE2	PHE	960	17.607	35.908	-12.296	1.00 18.22	6
ATOM	1041	CZ	PHE	960	16.777	35.415	-13.301	1.00 18.22	6
ATOM	1042	C	PHE	960	21.225	31.549	-10.402	1.00 48.69	6
ATOM	1043	0	PHE	960	21.203	30.329	-10.251	1.00 48.69	8
ATOM	1044	N	ILE	961	22.000	32.348	-9.674	1.00 25.93	7
ATOM	1045	CA	ILE	961	22.814	31.840	-8.561	1.00 25.93	6
ATOM	1046	CB	ILE	961	24.347	31.827	-8.883	1.00 5.00	6
ATOM	1047	CG2	ILE	961	25.140	31.201	-7.756	1.00 5.00	6
ATOM	1048	CG1	ILE	961	24.610	31.048	-10.132	1.00 5.00	6
ATOM	1049	CD1	ILE	961	25.990	31.281	-10.676	1.00 5.00	6
ATOM	1050	C	ILE	961	22.542	32.864	-7.449	1.00 25.93	6
ATOM	1051	0	ILE	961	22.658	34.061	~7.689	1.00 25.93	8
MOTA	1052	N	HIS	962	22.193	32.412	-6.247	1.00 38.00	7
ATOM	1053	CA	HIS	962	21.871	33.355	-5.180	1.00 38.00	6
ATOM	1054	CB	HIS	962	21.093	32.661	-4.072	1.00 25.73	6
ATOM	1055	CG	HIS	962	20.206	33.579	-3.289	1.00 25.73	6
ATOM	1056	CD2	HIS	962	20.482	34.461	-2.308	1.00 25.73	6
ATOM	1057	ND1	HIS	962	18.846	33.614	-3.475	1.00 25.73	7
ATOM	1058	CE1	HIS	962	18.315	34.478	-2.625	1.00 25.73	6
ATOM	1059		HIS	962	19.282	35.004	-1.903	1.00 25.73	7
ATOM	1060	С	HIS	962	23.054	34.079	-4.573	1.00 38.00	6
ATOM	1061	0	HIS	962	23.119	35.303	-4.637	1.00 38.00	8
ATOM	1062	N	ARG	963	23.972	33.338	-3.958	1.00 61.33	7
ATOM	1063	CA	ARG	963	25.152	33.932	-3.334	1.00 61.33	6
ATOM	1064	CB	ARG	963	25.855	34.907	-4.306	1.00 42.94	6
ATOM	1065	CG	ARG	963	25.864	34.466	-5.753	1.00 42.94	6
ATOM	1066	CD	ARG	963	26.986	35.078	-6.571	1.00 42.94	6
ATOM	1067	NE	ARG	963	26.799	36.481	-6.929	1.00 42.94	7
ATOM	1068	CZ	ARG	963	26.940	37.488	-6.929	1.00 42.94	6
ATOM	1069		ARG	963	27.268	37.258	-4.809	1.00 42.94	7
ATOM	1070		ARG	963	26.752	38.723	-6.508	1.00 42.94	7
ATOM	1071	C	ARG	963	24.756	34.688	-2.062	1.00 42.94	6
ATOM	1072	0	ARG	963	25.543	35.464	-1.528	1.00 61.33	8
		-			20.525	55.404	1.520	1.00 01.33	0

Inventors:

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Title: Method of Identifying Inhibitors of TIE-2

Nancy J. Bump et al.

23.549 34.460 -1.561 1.00 37.36 23.111 35.212 -0.384 1.00 37.36 22.742 36.636 -0.805 1.00 69.75 23.319 37.670 0.107 1.00 69.75 23.337 37.499 1.324 1.00 69.75 ATOM 1073 N ASN 964 ATOM 1074 CA ASN 964 1075 CB ASN 964 ATOM ATOM 1076 CG ASN 964 1077 OD1 ASN 964 ATOM ATOM 1078 ND2 ASN 964 23.792 38.761 -0.468 1.00 69.75 | 1079 | C ASN | 964 | 23.792 | 38.761 | -0.468 | 1.00 | 69.75 |
1080	O ASN	964	21.999	34.573	0.273	1.00	37.36	
1081	N LEU	965	21.812	33.258	0.133	1.00	45.72	
1082	CA LEU	965	20.691	32.503	0.666	1.00	45.72	
1083	CB LEU	965	20.515	31.230	-0.182	1.00	22.49	
1084	CG LEU	965	19.348	30.261	-0.002	1.00	22.49	
1085	CD1 LEU	965	19.348	30.261	-0.002	1.00	22.49	
1086	CD2 LEU	965	19.237	29.344	-1.189	1.00	22.49	
1086	CD2 LEU	965	19.565	29.461	1.252	1.00	22.49	
1087	C LEU	965	20.867	32.180	2.151	1.00	45.72	
1088	O LEU	965	20.867	32.180	2.151	1.00	45.72	
1089	N ALA	966	19.898	32.605	2.948	1.00	9.29	
1091	CB ALA	966	19.898	32.364	4.386	1.00	9.29	
1092	C ALA	966	18.474	32.615	4.891	1.00	9.29	
1093	O ALA	967	16.855	32.963	4.107	1.00	9.29	
1094	N ALA	967	16.855	32.698	6.627	1.00	20.93	
1096	CB ALA	967	16.855	32.698	6.672	1.00	20.93	
1097	CA ALA	967	16.855	32.698	6.672	1.00	20.93	
1098	O ALA	967	16.855	32.698	6.672	1.00	20.93	
1099	N ALA	967	15.355	34.486	6.393	1.00	20.93	
1099	N ALA	967	15.355	34.486	6.393	1.00	20.93	
1099	N ALA	967	15.355	34.486	6.393	1.00	20.93	
1099	N ALA	967	15.355	35.077	6.875	1.00	18.97	
1100	CA	ARG	968	17.423	35.077	6.875	1.00	18.97
1101	CB	ARG	968	19.596	36.932	6.747	1.00	55.21
1101	CD	ARG	968	19.596	36.932	6.747	1.00	55.21
1101	CD	ARG	968	19.596	36.932	6.747	1.00	55.21
1101	CD	ARG	968	20.653	38.006	6.946	1.00	55.21
1101	CD	ARG	968	20.653	38.006	6.946	1.00	55.21
1101	CD	ARG	968	20.653	38.006	6.946	1.00	55.21
1101	CD	ARG	968	20.653	38.006	6.946	1.00	55.21
1101	CD	ARG	968	ATOM 1079 C ASN 964 21.909 34.573 0.273 1.00 37.36 ATOM ATOM ATOM ATOM MOTA MOTA ATOM MOTA ATOM ATOM ATOM MOTA 6 MOTA 6 MOTA ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM MOTA 1103 CD ARG 968 20.653 38.006 6.946 1.00 55.21 MOTA 1104 NE ARG 968 21.881 37.608 6.275 1.00 55.21 1105 CZ ARG 968 ATOM 22.617 36.572 6.652 1.00 55.21 ATOM 1106 NH1 ARG 968 22.246 35.846 7.704 1.00 55.21 ATOM 1107 NH2 ARG 968 5.954 1.00 55.21 23.697 36.244 7 ATOM 1108 C ARG 968 16.632 37.016 5.548 1.00 18.97 15.790 37.915 5.477 1.00 18.97 17.165 36.427 4.481 1.00 17.09 ATOM 1109 O ARG 968 ATOM 1110 N ASN 969 7 1111 CA ASN 969 MOTA 16.820 36.815 3.109 1.00 17.09 2.179 1.00 47.15 1112 CB ASN 969 MOTA 18.008 36.589 1113 CG ASN 969 ATOM 19.028 37.700 2.240 1.00 47.15 ATOM MOTA ATOM ATOM ATOM ATOM ATOM 6 MOTA 6 ATOM ATOM 14.542 32.175 1.313 1.00 5.00 6 ATOM 1124 C ILE 970 12.395 35.687 3.653 1.00 17.16 ATOM 1125 O ILE 970 12.395 35.687 3.653 1.00 17.16 ATOM 1126 N LEU 971 12.454 35.923 4.864 1.00 17.16 ATOM 1126 N LEU 971 11.365 36.047 2.903 1.00 27.06 ATOM 1127 CA LEU 971 10.234 36.784 3.443 1.00 27.06 ATOM 1128 CB LEU 971 10.000 38.039 2.584 1.00 23.00 ATOM 1129 CG LEU 971 11.152 39.063 2.585 1.00 23.00 7				

Docket/App No.: 2079.1037-001

Title: Method of Identifying Inhibitors of TIE-2 Nancy J. Bump et al. Inventors:

ATOM 1130 CD1 LEU 971 11.197 39.762 1.249 1.00 23.00 ATOM 1131 CD2 LEU 971 10.990 40.054 3.689 1.00 23.00 3.465 1.00 27.06 ATOM 1132 C LEU 971 8.984 35.910 ATOM 1133 LEU 971 8,730 35.192 2.511 1.00 27.06 0 ATOM 1134 N VAL 972 8.218 35.967 4.558 1.00 35.27 972 ATOM 1135 CA VAL 6.974 35.188 4.710 1.00 35.27 CB 972 6.641 34.916 6.237 1.00 15.12 ATOM 1136 VAL 972 ATOM 1137 CG1 VAL 5.384 34.069 6.387 1.00 15.12 ATOM 1138 CG2 VAL 972 7.806 34.239 6.917 1.00 15.12 972 4.086 1.00 35.27 ATOM 1139 C VAL 5.805 35.979 972 ATOM 1140 0 VAT. 5.220 36.848 4.727 1.00 35.27 ATOM 1141 N GLY 973 5.466 35.686 2.841 1.00 28.86 ATOM 1142 CA GLY 973 4.378 36.404 2.212 1.00 28.86 ATOM 1143 C GLY 973 3.021 35.983 2.743 1.00 28.86 ATOM 1144 0 GLY 973 2.933 35.251 3.734 1.00 28.86 ATOM 1145 N GLU 974 2.092 1.00 36.97 1.954 36.429 ATOM 1146 CA GLU 974 0.621 36.081 2.554 1.00 36.97 1147 CB GLU 974 -0.434 36.662 1.619 1.00 98.72 ATOM 1148 CG GLU 974 ATOM -1.001 37.980 2.107 1.00 98.72 1149 CD GLU 974 -1.619 37.873 3.503 1.00 98.72 ATOM ATOM 1150 OE1 GLU 974 -2.364 36.904 3.759 1.00 98.72 4.342 1.00 98.72 ATOM 1151 OE2 GLU 974 -1.368 38.763 GLU . 974 2.720 1.00 36.97 ATOM 1152 C 0.418 34.585 ATOM 1153 0 GLU 974 1.049 33.768 2.034 1.00 36.97 ATOM 1154 N ASN 975 -0.474 34.253 3.649 1.00 50.17 ATOM 1155 CA ASN 975 -0.811 32.878 3.980 1.00 50.17 1156 CB ASN 975 ATOM -1.496 32.190 2.812 1.00 49.51 ATOM 1157 CG ASN 975 -2.900 32.725 2.577 1.00 49.51 ATOM 1158 OD1 ASN 975 -3.688 32.145 1.834 1.00 49.51 ATOM 1159 ND2 ASN 975 -3.218 33.851 3.213 1.00 49.51 ATOM 1160 C ASN 975 0.432 32.122 4.392 1.00 50.17 ATOM 1161 0 ASN 975 0.528 30.910 4.222 1.00 50.17 ATOM 1162 N 976 4.931 1.00 34.67 TYR 1.386 32.871 ATOM 1163 CA TYR 976 5.427 1.00 34.67 2.637 32.335 ATOM 1164 CB TYR 976 2.386 31.613 6.734 1.00 32.84 ATOM 976 7.736 1.00 32.84 1165 CG TYR 1.690 32.497 ATOM 1166 CD1 TYR 976 0.309 32.654 7.715 1.00 32.84 ATOM 1167 CE1 TYR 976 -0.328 33.464 8.625 1.00 32.84 ATOM 1168 CD2 TYR 976 2.411 33.182 8.693 1.00 32.84 ATOM 1169 CE2 TYR 976 1.792 33.991 9.602 1.00 32.84 ATOM 1170 CZ TYR 976 0.422 34.129 9.571 1.00 32.84 1171 OH TYR -0.210 34.897 ATOM 976 10.515 1.00 32.84 ATOM 1172 976 4.475 1.00 34.67 C TYR 3.376 31.440 4.875 1.00 34.67 ATOM 1173 TYR 976 3.903 30.410 0 1174 N 3.217 1.00 16.20 ATOM VAL 977 3.436 31.857 2.181 1.00 16.20 ATOM 1175 CA VAL 977 4.135 31.111 ATOM VAL 0.876 1.00 9.07 1176 CB 977 3.297 31.091 ATOM 1177 CG1 VAL 977 4.187 30.767 -0.331 1.00 9.07 1.005 1.00 9.07 MOTA 1178 CG2 VAL 977 2.153 30.102 ATOM 1179 C VAL 977 5.490 31.755 1.900 1.00 16.20 1180 O 1.284 1.00 16.20 ATOM VAL 977 5.545 32.795 ATOM 1181 N ALA 978 6.571 31.126 2.337 1.00 15.88 ATOM 1182 CA ALA 978 7.924 31.643 2.141 1.00 15.88 ATOM 1183 CB ALA 978 8.940 30.547 2.489 1.00 21.88 ATOM 1184 C ALA 978 8.238 32.215 0.757 1.00 15.88 ATOM 1185 0 ALA 978 7.905 31.630 -0.268 1.00 15.88 ATOM 1186 N LYS 979 8.920 0.736 1.00 28.57 33.352

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	ATOM	1187	CA	LYS	979	9.284	34.011	-0.508	1.00 28.57	6
	MOTA	1188	CB	LYS	979	8.468	35.289	-0.621	1.00 15.51	6
	MOTA	1189	CG	LYS	979	6.969	35.078	-0.838	1.00 15.51	6
	ATOM	1190	CD	LYS	979	6.698	34.786	-2.297	1.00 15.51	6
	ATOM	1191	CE	LYS	979	5.254	35.044	-2.662	1.00 15.51	6
	ATOM	1192	NZ	LYS	979	4.388	34.606	-1.545	1.00 15.51	7
	ATOM	1193	C	LYS	979	10.800	34.294	-0.506	1.00 28.57	6
	ATOM	1194	0	LYS	979	11.348	34.679	0.525	1.00 28.57	8
	ATOM	1195	N	ILE	980	11.458	34.082	-1.655	1.00 23.28	7
	ATOM	1196	CA	ILE	980	12.914	34.271	-1.815	1.00 23.28	6
	ATOM	1197	CB	ILE	980	13.507	33.236	-2.812	1.00 12.16	6
	ATOM	1198	CG2	ILE	980	14.986	33.535	-3.046	1.00 12.16	6
	MOTA	1199	CG1	ILE	980	13.309	31.804	-2.268	1.00 12.16	6
	MOTA	1200	CD1	ILE	980	13.475	30.688	-3.319	1.00 12.16	6
	MOTA	1201	С	ILE	980	13.270	35.665	-2.301	1.00 23.28	6
	ATOM	1202	0	ILE	980	12.739	36.135	-3.292	1.00 23.28	8
	MOTA	1203	N	ALA	981	14.185	36.335	-1.623	1.00 30.98	7
	ATOM	1204	CA	ALA	981	14.538	37.683	-2.040	1.00 30.98	6
	MOTA	1205	CB	ALA	981	13.810	38.664	-1.156	1.00 12.02	6
	ATOM	1206	C	ALA	981	16.047	37.959	-2.021	1.00 30.98	6
(3	ATOM	1207	0	ALA	981	16.840	37.172	-1.499	1.00 30.98	8
1/2	ATOM	1208	N	ASP	982	16.433	39.094	-2.589	1.00 70.73	7
00	ATOM	1209	CA	ASP	982	17.834	39.511	-2.652	1.00 70.73	6
500	ATOM	1210	CB	ASP	982	18.327	39.939	-1.272	1.00 99.58	6
131	ATOM	1211	CG	ASP	982	19.512	40.861	-1.358	1.00 99.58	6
	MOTA	1212		ASP	982	19.287	42.012	-1.783	1.00 99.58	8
42	MOTA	1213		ASP	982	20.646	40.436	-1.039	1.00 99.58	8
Las.	ATOM	1214	C	ASP	982	18.821	38.488	-3.199	1.00 70.73	6
	ATOM	1215	0	ASP	982	19.686	38.005	-2.477	1.00 70.73	8
SE COMM	ATOM	1216	N	PHE	983	18.703	38.184	-4.479	1.00 67.82	7
	MOTA	1217	CA	PHE	983	19.595	37.229	-5.095	1.00 67.82	6
LA!	ATOM	1218	CB	PHE	983	18.781	36.124	-5.784	1.00 46.69	6
TU	MOTA	1219	CG	PHE	983	17.480	36.593	-6.382	1.00 46.69	6
13.	ATOM	1220		PHE	983	17.423	37.752	-7.143	1.00 46.69	6
-	MOTA	1221		PHE	983	16.317	35.852	-6.222	1.00 46.69	6
in the	ATOM	1222		PHE	983	16.229	38.166	-7.737	1.00 46.69	6
	MOTA	1223	CE2	PHE	983	15.122	36.259	-6.814	1.00 46.69	6
	MOTA	1224	CZ	PHE	983	15.080	37.413	-7.570	1.00 46.69	6
	ATOM	1225	C	PHE	983	20.552	37.905	-6.081	1.00 67.82	6
	ATOM	1226	0	PHE	983	20.451	39.112	-6.338	1.00 67.82	8
	ATOM	1227	N	GLY	984	21.497	37.128	-6.599	1.00 44.02	7
	ATOM	1228	CA	GLY	984	22.467	37.644	-7.543	1.00 44.02	6
	MOTA	1229	C	GLY	984	21.911	37.639	-8.954	1.00 44.02	6
	MOTA	1230	0	GLY	984	21.520	36.599	-9.488	1.00 44.02	8
	ATOM	1231	N	LEU	985	21.875	38.816	-9.562	1.00100.00	7
	ATOM	1232	CA	LEU	985	21.363	38.951	-10.917	1.00100.00	6
	ATOM	1233	CB	LEU	985	20.792	40.360	-11.126	1.00 41.04	6
	ATOM	1234	CG	LEU	985	19.455		-10.434	1.00 41.04	6
	ATOM	1235		LEU	985	18.448	39.621	-10.945	1.00 41.04	6
	ATOM	1236		LEU	985	19.577	40.549	-8.925	1.00 41.04	6
	ATOM	1237	C	LEU	985	22.473		-11.920	1.00100.00	6
	MOTA	1238	0	LEU	985	22.517		-13.004	1.00100.00	8
	MOTA	1239	N	SER	986	23.383		-11.539	1.00 42.70	7
	ATOM	1240	CA	SER	986	24.484		-12.416	1.00 42.70	6
	ATOM	1241	CB	SER	986	25.818		-11.697	1.00 68.70	6
	MOTA	1242	OG	SER	986	25.996		-11.346	1.00 68.70	8
	ATOM	1243	C	SER	986	24.295	35.955	-12.780	1.00 42.70	6

ATOM	1244	0	SER	986	24.956	35.078	-12.238	1.00 42.70	8
ATOM	1245	N	ARG	987	23.381	35.697	-13.703	1.00 47.12	7
ATOM	1246	CA	ARG	987	23.068	34.336	-14.124	1.00 47.12	6
ATOM	1247	CB	ARG	987	21.873	34.383	-15.045	1.00 55.43	6
ATOM	1248	CG	ARG	987	20.828	35.354		1.00 55.43	6
ATOM	1249	CD	ARG	987	19.927	35.581		1.00 55.43	6
ATOM	1250	NE	ARG	987	19.371	34.311		1.00 55.43	7
	1251	CZ	ARG	987	18.891	34.116		1.00 55.43	6
ATOM	1251		ARG	987	18.924		-18.261	1.00 55.43	7
ATOM	1252		ARG	987	18.364	32.946		1.00 55.43	7
ATOM	1254	C	ARG	987	24.204	33.608		1.00 47.12	6
ATOM	1255	0	ARG	987	24.990	34.223		1.00 47.12	8
ATOM	1255	N	GLY	988	24.281	32.294		1.00 32.39	7
ATOM		CA	GLY	988	25.330	31.512		1.00 32.39	6
ATOM	1257	CA	GLY	988	25.704		-14.592	1.00 32.39	6
ATOM	1258	0	GLY	988	24.832	29.393		1.00 32.39	8
MOTA	1259		GLN	989	26.999	29.978		1.00 53.32	7
ATOM	1260	N	GLN	989	27.473		-13.738	1.00 53.32	6
ATOM	1261	CA		989	28.063		-14.761	1.00 52.63	6
ATOM	1262	CB	GLN	989	27.056		-15.207	1.00 52.63	6
ATOM	1263	CG	GLN	989	27.583		-15.120	1.00 52.63	6
ATOM	1264	CD	GLN	989	28.219		-16.052	1.00 52.63	8
MOTA	1265		GLN	989	27.355		-13.985	1.00 52.63	7
ATOM	1266		GLN	989	28.473		-12.631	1.00 53.32	6
ATOM	1267 1268	C	GLN	989	28.683		-11.861	1.00 53.32	8
ATOM		NI.	GLU	990	29.082		-12.532	1.00 57.00	7
ATOM	1269 1270	CA	GLU	990	30.072		-11.503	1.00 57.00	6
ATOM	1270	CB	GLU	990	31.320		-11.858	1.00 60.46	6
ATOM ATOM	1271	CG	GLU	990	32.281		-10.745	1.00 60.46	6
ATOM	1272	CD	GLU	990	32.976	27.979	-10.927	1.00 60.46	6
ATOM	1274		GLU	990	33.448	27.718	-12.049	1.00 60.46	8
ATOM	1274		GLU	990	33.044	27.198	-9.960	1.00 60.46	В
ATOM	1276	C	GLU	990	30.368	31.814	-11.523	1.00 57.00	6
ATOM	1277	Ö	GLU	990	30.639	32.363	-12.589	1.00 57.00	8
ATOM	1278	N	VAL	991	30.269	32.470	-10.367	1.00 47.34	7
ATOM	1279	CA	VAL	991	30.567	33.904	-10.285	1.00 47.34	6
ATOM	1280	CB	VAL	991	29.423	34.745	-9.575	1.00 25.98	6
ATOM	1281		VAL	991	29.646	36.247	-9.822	1.00 25.98	6
ATOM	1282	CG2		991	28.029	34.365	-10.094	1.00 25.98	6
ATOM	1283	C	VAL	991	31.878	34.057	-9.493	1.00 47.34	6
ATOM	1284	0	VAL	991	32.387	33.090	-8.924	1.00 47.34	8
ATOM	1285	N	TYR	992	32.437	35.262	-9.483	1.00 68.84	7
ATOM	1286	CA	TYR	992	33.683	35.517	-8.774	1.00 68.84	6
ATOM	1287	CB	TYR	992	34.849	35.554	-9.765	1.00 49.61	6
ATOM	1288	CG	TYR	992	36.187	35.817	-9.103	1.00 49.61	6
ATOM	1289	CD:	1 TYR	992	36.680	34.950	-8.127	1.00 49.61	6
ATOM	1290	CE:	1 TYR	992	37.886	35.201	-7.465	1.00 49.61	6
ATOM	1291	CD:	2 TYR	992	36.941	36.947	-9.410	1.00 49.61	6
ATOM	1292	CE:	2 TYR	992	38.154	37.210		1.00 49.61	6
ATOM	1293	CZ	TYR	992	38.614	36.333	-7.780	1.00 49.61	6
ATOM	1294	OH	TYR	992	39.785	36.607		1.00 49.61	8
ATOM	1295	C	TYR	992	33.653	36.836		1.00 68.84	6
MOTA	1296	0	TYR	992	33.941	37.886		1.00 68.84	8
ATOM	1297	N	VAL	993	33.312	36.802		1.00 73.45	7
ATOM	1298	CA	VAL	993	33.293	38.048		1.00 73.45	6
ATOM	1299	CB	VAL	993	32.078	38.110		1.00 77.88	6
ATOM	1300	CG	1 VAL	993	30.812	38.28	L -5.857	1.00 77.88	6

COMMINIAL DIFFERENCE

FIG. 3W ~

ATOM	1301	CG2	VAL	993	32.012	36.866	-4.236	1.00 77.88	6
ATOM	1302	C	VAL	993	34.585	38.227	~5.162	1.00 73.45	6
ATOM	1303	0	VAL	993	35.222	37.248	-4.762	1.00 73.45	8
ATOM	1304	N	LYS	994	34.965	39.483	-4.946	1.00100.00	7
ATOM	1305	CA.	LYS	994	36.190		-4.225	1.00100.00	6
ATOM	1306	CB	LYS	994	37.340	39.934	-5.227	1.00 96.49	6
ATOM	1307	CG	LYS	994	38.693	40.258	-4.635	1.00 96.49	6
ATOM	1308	CD	LYS	994	39.679	40.656	-5.728	1.00 96.49	6
ATOM	1309	CE	LYS	994	40.977	39.891	-5.576	1.00 96.49	6
ATOM	1310	NZ	LYS	994	41.937	40.208	-6.655	1.00 96.49	7
ATOM	1311	C	LYS	994	35.981	41.170	-3.525	1.00100.00	6
ATOM	1312	ō	LYS	994	36.298	42.217	-4.089	1.00100.00	8
		N	LYS	995	35.456	41.135	-2.299	1.00100.00	7
ATOM	1313		LYS	995	35.173		-1.505	1.00100.00	6
ATOM	1314	CA					-1.423	1.00100.00	6
ATOM	1315	CB	LYS	995	36.432	43.233		1.00100.00	6
ATOM	1316	C	LYS	995	33.996		-2.094		
MOTA	1317	0	LYS	995	34.079		-2.139	1.00100.00	8
ATOM TER	1318	OXT	LYS	995	33.001	42.485	-2.484	1.00 85.30	8
ATOM	1319	CB	PRO	1001	26.968	35.804	4.979	1.00 23.69	6
ATOM	1320	CG	PRO	1001	26.527	36.525	3.738	1.00 23.69	6
ATOM	1321	C	PRO	1001	29.219	34.895	5.215	1.00 43.97	6
ATOM	1322	0	PRO	1001	28.910	33.885	4.598	1.00 43.97	8
ATOM	1323	N	PRO	1001	28.835	36.609	3.692	1.00 43.97	7
ATOM	1324	CD	PRO	1001	27.692	36.488	2.779	1.00 23.69	6
ATOM	1325	CA	PRO	1001	28.434	36.157	5.028	1.00 43.97	6
ATOM	1326	N	VAL	1002	30.217	34.937	6.077	1.00 30.46	7
ATOM	1327	CA	VAL	1002	31.040	33.763	6.267	1.00 30.46	6
ATOM	1328	CB	VAL	1002	32.241	34.137	7.118	1.00 49.80	6
ATOM	1329	CG1	VAL	1002	32.805	35.456	6.632	1.00 49.80	6
ATOM	1330	CG2	VAL	1002	31.852	34.219	8.578	1.00 49.80	6
ATOM	1331	С	VAL	1002	30.360	32.503	6.834	1.00 30.46	6
ATOM	1332	0	VAL	1002	30.790	31.389	6.553	1.00 30.46	8
ATOM	1333	N	ARG	1003	29.292		7.596	1.00 40.35	7
ATOM	1334	CA	ARG	1003	28.643		8.207	1.00 40.35	6
ATOM	1335	CB	ARG	1003	27.872		9.444	1.00 42.33	6
ATOM	1336	CG	ARG	1003	28.755		10.626	1.00 42.33	6
ATOM	1337	CD	ARG	1003	27.857		11.767	1.00 42.33	6
ATOM	1338	NE	ARG	1003	28.533		13.047	1.00 42.33	7
ATOM	1339	CZ	ARG	1003	29.508		13.336	1.00 42.33	6
ATOM	1340		ARG	1003	29.932		12.428	1.00 42.33	7
ATOM	1341		ARG	1003	30.067		14.535	1.00 42.33	7
ATOM	1342	C	ARG	1003	27.737		7.370	1.00 40.35	6
ATOM	1342	0	ARG	1003	27.262		7.865	1.00 40.35	8
ATOM	1343	N	TRP	1003	27.495		6.121	1.00 26.04	7
ATOM	1344	CA	TRP	1004	26.632		5.221	1.00 26.04	6
							4.768	1.00 50.68	6
ATOM	1346	CB	TRP	1004	25.459		5.776	1.00 50.68	6
ATOM	1347	CG	TRP	1004	24.332				6
ATOM	1348	CD2		1004	24.26		6.885	1.00 50.68	
MOTA	1349	CE2		1004	23.066		7.585	1.00 50.68	6
ATOM	1350	CE3		1004	25.093		7.363	1.00 50.68	
MOTA	1351	CD1		1004	23.20		5.843	1.00 50.68	6 7
ATOM	1352		TRP	1004	22.445		6.924	1.00 50.68	
ATOM	1353	CZ2		1004	22.683		8.737	1.00 50.68	6
ATOM	1354	CZ3		1004	24.70		8.515	1.00 50.68	6
ATOM	1355	CH2		1004	23.51			1.00 50.68	6
ATOM	1356	С	TRP	1004	27.40	9 29.747	4.006	1.00 26.04	6

TORALDIA DUBLIA

Title: Method of Identifying Inhibitors of TIE-2 Inventors: Nancy J. Bump *et al.*

ATOM 1357 0 TRP 1004 27.003 28.794 3.356 1.00 26.04 MET 1005 ATOM 1358 N 28.535 30.382 3.706 1.00 37.80 ATOM 1359 CA MET 1005 29.329 30.009 2.543 1.00 37.80 1360 CB MET 1005 30.502 30.949 2.412 1.00 40.16 ATOM ATOM 1361 CG MET 1005 30.063 32.299 1.973 1.00 40.16 1362 SD MET 1005 ATOM 31.319 33.493 2.212 1.00 40.16 16 MOTA 1363 CE MET 1005 32.621 32.780 1.246 1.00 40.16 ATOM 1364 C MET 1005 29.827 28.584 2.473 1.00 37.80 ATOM 1365 0 MET 1005 30.268 28.011 3.465 1.00 37.80 ALA 1006 29.753 28.008 1.283 1.00 45.98 ATOM 1366 N 1367 CA ALA 1006 30.230 26.654 MOTA 1.092 1.00 45.98 ATOM 1368 CB ALA 1006 29.797 26.138 -0.284 1.00 10.86 31.764 26.736 ALA 1006 1.196 1.00 45.98 ATOM 1369 C ATOM 1370 0 ALA 1006 32.322 27.830 1.151 1.00 45.98 1.326 1.00 44.58 MOTA 1371 N ILE 1007 32.448 25.604 1372 CA ILE 1007 ATOM 33.909 25.657 1.446 1.00 44.58 6 ATOM 1373 CB ILE 1007 34.528 24.267 1.753 1.00 25.13 ATOM 1374 CG2 ILE 1007 34.415 23.969 3.224 1.00 25.13 ATOM 1375 CG1 ILE 1007 33.880 23.182 0.886 1.00 25.13 ATOM 1376 CD1 ILE 1007 34.418 23.123 -0.571 1.00 25.13 ATOM 1377 C ILE 1007 34.619 26.244 0.234 1.00 44.58 ATOM 1378 0 ILE 1007 35.585 26.988 0.379 1.00 44.58 ATOM 1379 N GLU 1008 34.137 25.915 -0.957 1.00 31.07 ATOM 1380 CA GLU 1008 34.743 26.402 -2.188 1.00 31.07 1381 CB GLU 1008 ATOM 34.089 25.710 -3.378 1.00 43.81 ATOM 1382 CG GLU 1008 32.595 25.941 -3.415 1.00 43.81 ATOM 1383 CD GLU 1008 31.795 24.661 -3.241 1.00 43.81 ATOM 1384 OE1 GLU 1008 31.967 23.953 -2.216 1.00 43.81 1385 OE2 GLU 1008 30.965 24.377 ATOM -4.125 1.00 43.81 ATOM 1386 C GLU 1008 34.578 27.914 35.377 28.583 -2.308 1.00 31.07 1387 0 GLU 1008 ATOM -2.967 1.00 31.07 1388 N SER 1009 33.546 28.447 ATOM -1.660 1.00 30.15 ATOM 1389 CA SER 1009 33.259 29.873 -1.711 1.00 30.15 6 ATOM 1390 CB SER 1009 31.802 30.117 -1.366 1.00 23.09 6 ATOM 1391 OG SER 1009 30.984 29.174 -2.034 1.00 23.09 B ATOM 1392 C SER 1009 34.150 30.622 -0.743 1.00 30.15 ATOM 1393 0 SER 1009 34.565 31.760 -0.995 1.00 30.15 MOTA 1394 N LEU 1010 34.428 29.977 0.381 1.00 29.90 MOTA 1395 CA LEU 1010 35.293 30.566 1.380 1.00 29.90 ATOM 1396 CB LEU 1010 35.402 29.629 2.585 1.00 44.65 ATOM 1397 CG LEU 1010 34.152 29.450 3.460 1.00 44.65 ATOM 1398 CD1 LEU 1010 34.435 28.420 4.534 1.00 44.65 6 ATOM 1399 CD2 LEU 1010 33.752 30.781 4.101 1.00 44.65 ATOM 1400 C LEU 1010 36.663 30.771 0.726 1.00 29.90 ATOM 1401 0 LEU 1010 37.082 31.912 0.503 1.00 29.90 Я ATOM 1402 N ASN 1011 37.327 29.661 0.397 1.00 34.23 ATOM 1403 CA ASN 1011 38.652 29.638 -0.230 1.00 34.23 ATOM 1404 CB ASN 1011 39.105 28.205 -0.511 1.00 32.72 ATOM 1405 CG ASN 1011 38.990 27.287 0.679 1.00 32.72 ATOM 1406 OD1 ASN 1011 39.433 27.600 1.783 1.00 32.72 MOTA 1407 ND2 ASN 1011 38.404 26.117 0.450 1.00 32.72 -1.560 1.00 34.23 ATOM 1408 C ASN 1011 38.801 30.353 6 ATOM 1409 0 ASN 1011 39.728 31.137 -1.748 1.00 34.23 8 1410 N TYR 1012 ATOM 37.914 30.041 -2.494 1.00 35.06 1411 CA TYR 1012 ATOM 38.018 30.611 -3.822 1.00 35.06 ATOM 1412 CB TYR 1012 37.824 29.521 -4.845 1.00 40.77

ATOM

1413 CG TYR 1012

38.705 28.358 -4.552 1.00 40.77

for.

ATOM	1414	CD1	TYR	1012	38.167	27.093	-4.400	1.00 40.77	6
ATOM	1415	CEI		1012	38.961	26.024	-4.105	1.00 40.77	6
ATOM	1416	CD2	TYR	1012	40.077	28.531	-4.397	1.00 40.77	6
ATOM	1417	CE2	TYR	1012	40.896	27.472	-4.098	1.00 40.77	6
MOTA	1418	CZ	TYR	1012	40.336	26.208	-3.957	1.00 40.77	6
ATOM	1419	OH	TYR	1012	41.152	25.119	-3.717	1.00 40.77	8
MOTA	1420	C	TYR	1012	37.161	31.787	-4.193	1.00 35.06	6
MOTA	1421	0	TYR	1012	37.443	32.440	-5.195	1.00 35.06	8
ATOM	1422	N	SER	1013	36.109	32.060	-3.433	1.00 42.36	7
ATOM	1423	CA	SER	1013	35.278	33.209	-3.746	1.00 42.36	6
ATOM	1424	CB	SER	1013	36.159	34.439	-3.983	1.00 39.37	6
ATOM	1425	OG	SER	1013	37.157	34.576	-2.983	1.00 39.37	8
ATOM	1426	C	SER	1013	34.433	32.973	-4.982	1.00 42.36	6
ATOM	1427	0	SER	1013	34.291	33.865	-5.807	1.00 42.36	8
MOTA	1428	N	VAL	1014	33.890	31.772	-5.121	1.00 22.55	7
ATOM	1429	CA	VAL	1014	33.045	31.467	-6.260	1.00 22.55	6
ATOM	1430	CB	VAL	1014	33.653	30.369	-7.143	1.00 31.51	6
MOTA	1431	CG1	VAL	1014	35.048	30.791	-7.599	1.00 31.51	6
ATOM	1432	CG2	VAL	1014	33.701	29.054	-6.383	1.00 31.51	6
ATOM	1433	C	VAL	1014	31.720	30.999	-5.712	1.00 22.55	6
ATOM	1434	0	VAL	1014	31.644	30.562	-4.577	1.00 22.55	8
ATOM	1435	N	TYR	1015	30.671	31.121	-6.507	1.00 26.01	7
ATOM	1436	CA	TYR	1015	29.338	30.712	-6.101	1.00 26.01	6
ATOM	1437	CB	TYR	1015	28.501	31.938	-5.753	1.00 41.40	6
ATOM	1438	CG	TYR	1015	29.116	32.782	-4.672	1.00 41.40	6
MOTA	1439	CD1	TYR	1015	30.233	33.560	-4.922	1.00 41.40	6
ATOM	1440	CE1	TYR	1015	30.854	34.235	-3.904	1.00 41.40	6
ATOM	1441	CD2	TYR	1015	28.638	32.709	-3.365	1.00 41.40	6
ATOM	1442	CE2	TYR	1015	29.257	33.388	-2.330	1.00 41.40	6
ATOM	1443	CZ	TYR	1015	30.361	34.139	-2.605	1.00 41.40	6
ATOM	1444	OH	TYR	1015	30.968	34.830	-1.588	1.00 41.40	8
ATOM	1445	C	TYR	1015	28.674	29.998	-7.252	1.00 26.01	6
ATOM	1446	0	TYR	1015	28.513	30.572	-8.324	1.00 26.01	8
ATOM	1447	N	THR	1016	28.311	28.741	-7.043	1.00 17.46	7
ATOM	1448	CA	THR	1016	27.610	27.971	-8.082	1.00 17.46	6
ATOM	1449	CB	THR	1016	28.317	26.625	-8.456	1.00 15.11	6
MOTA	1450	OG1	THR	1016	28.649	25.909	-7.262	1.00 15.11	8
MOTA	1451	CG2	THR	1016	29.540	26.855	-9.283	1.00 15.11	6
ATOM	1452	C	THR	1016	26.257	27.590	-7.487	1.00 17.46	6
ATOM	1453	0	THR	1016	25.919	28.038	-6.408	1.00 17.46	8
ATOM	1454	N	THR	1017	25.489	26.752	-8.171	1.00 10.55	7
MOTA	1455	CA	THR	1017	24.229	26.325	-7.585	1.00 10.55	6
ATOM	1456	CB	THR	1017	23.346	25.602	-8.600	1.00 29.18	6
ATOM	1457	OG1	THR	1017	22.913	26.533	-9.600	1.00 29.18	8
MOTA	1458	CG2	THR	1017	22.138	25.017	-7.906	1.00 29.18	6
ATOM	1459	C	THR	1017	24.563	25.381	-6.419	1.00 10.55	6
ATOM	1460	0	THR	1017	23.802	25.287	-5.466	1.00 10.55	8
ATOM	1461	N	ASN	1018	25.740	24.743	-6.500	1.00 41.35	7
ATOM	1462	CA	ASN	1018	26.266	23.772	-5.505	1.00 41.35	6
MOTA	1463	CB	ASN	1018	27.522	23.095	-6.033	1.00 49.00	6
ATOM	1464	CG	ASN	1018	27.234	22.010	-7.015	1.00 49.00	6
MOTA	1465	OD1	ASN	1018	28.100	21.630	-7.788	1.00 49.00	8
ATOM	1466	ND2	ASN	1018	26.025	21.477	-6.981	1.00 49.00	7
ATOM	1467	C	ASN	1018	26.646	24.371	-4.156	1.00 41.35	6
MOTA	1468	0	ASN	1018	26.773	23.647	-3.160	1.00 41.35	8
ATOM	1469	N	SER	1019	26.887	25.680	-4.148	1.00 46.21	7
MOTA	1470	CA	SER	1019	27.247	26.400	-2.935	1.00 46.21	6
								10.21	~

ATOM	1471	CB	SER	1019	28.179	27.570	-3.247	1.00 35.31	6
ATOM	1472	OG	SER	1019	27.517	28.561	-3.996	1.00 35.31	8
ATOM	1473	C	SER	1019	25.936	26.919	-2.392	1.00 46.21	6
ATOM	1474	0	SER	1019	25.835	27.281	-1.225	1.00 46.21	8
ATOM	1475	N	ASP	1020	24.929	26.965	-3.253	1.00 42.68	7
ATOM	1476	CA	ASP	1020	23.640	27.426	-2.808	1.00 42.68	6
ATOM	1477	CB	ASP	1020	22.826	28.008	-3.951	1.00 34.86	6
ATOM	1478	CG	ASP	1020	22.962	29.508	-4.032	1.00 34.86	6
ATOM	1479	OD1		1020	23.242	30.127	-2.972	1.00 34.86	8
ATOM	1480	OD2	ASP	1020	22.788	30.046	-5.149	1.00 34.86	8
ATOM	1481	С	ASP	1020	22.912	26.281	-2.171	1.00 42.68	6
ATOM	1482	ō	ASP	1020	21.925	26.487	-1.480	1.00 42.68	8
ATOM	1483	N	VAL	1021	23.401	25.071	-2.398	1.00 33.68	7
ATOM	1484	CA	VAL	1021	22.751	23.944	-1.787	1.00 33.68	6
ATOM	1485	CB	VAL	1021	22.872	22.690	-2.628	1.00 9.47	6
ATOM	1486		VAL	1021	22.096	21.575	-1.962	1.00 9.47	6
ATOM	1487		VAL	1021	22.328	22.940	-4.008	1.00 9.47	6
ATOM	1488	C	VAL	1021	23.403	23.746	-0.444	1.00 33.68	6
ATOM	1489	o	VAL	1021	22.872	23.740	0.422	1.00 33.68	8
ATOM	1490	N	TRP	1021	24.565	24.355	-0.268	1.00 49.04	7
ATOM	1491	CA	TRP	1022	25.247	24.333	1.011	1.00 49.04	6
ATOM	1491	CB	TRP	1022		24.204	0.868	1.00 36.23	6
ATOM	1492	CG			26.732			1.00 36.23	6
			TRP	1022	27.463	24.712	2.164		
ATOM	1494		TRP	1022	28.575	23.920	2.583	1.00 36.23	6
ATOM	1495	CE2	TRP	1022	28.985	24.411	3.836	1.00 36.23	6
ATOM	1496		TRP	1022	29.269	22.843	2.019	1.00 36.23	6
ATOM	1497		TRP	1022	27.246	25.623	3.158	1.00 36.23	6
ATOM	1498		TRP	1022	28.155	25.452	4.165	1.00 36.23	7
ATOM	1499	CZ2	TRP	1022	30.061	23.862	4.532	1.00 36.23	6
ATOM	1500		TRP	1022	30.338	22.300	2.710	1.00 36.23	6
ATOM	1501		TRP	1022	30.721	22.808	3.951	1.00 36.23	6
ATOM	1502	C	TRP	1022	24.558	25.391	1.777	1.00 49.04	6
ATOM	1503	0	TRP	1022	23.962	25.164	2.822	1.00 49.04	8
ATOM	1504	N	SER	1023	24.599	26.598	1.244	1.00 20.71	7
ATOM	1505	CA	SER	1023	23.946	27.666	1.954	1.00 20.71	6
ATOM	1506	CB	SER	1023	24.032	28.977	1.181	1.00 17.98	6
ATOM	1507	OG	SER	1023	25.377	29.363	1.081	1.00 17.98	8
ATOM	1508	C	SER	1023	22.516	27.305	2.265	1.00 20.71	6
ATOM	1509	0	SER	1023	22.009	27.705	3.298	1.00 20.71	8
ATOM	1510	N	TYR	1024	21.842	26.557	1.400	1.00 27.47	7
ATOM	1511	CA	TYR	1024	20.474	26.200	1.758	1.00 27.47	6
ATOM	1512	CB	TYR	1024	19.728	25.580	0.590	1.00 25.94	6
ATOM	1513	CG	TYR	1024	18.447	24.902	1.003	1.00 25.94	6
ATOM	1514	CD1	TYR	1024	17.222	25.512	0.847	1.00 25.94	6
ATOM	1515	CE1	TYR	1024	16.037	24.846	1.170	1.00 25.94	6
ATOM	1516	CD2	TYR	1024	18.465	23.611	1.506	1.00 25.94	6
ATOM	1517	CE2	TYR	1024	17.288	22.954	1.833	1.00 25.94	6
ATOM	1518	CZ	TYR	1024	16.089	23.579	1.656	1.00 25.94	6
ATOM	1519	OH	TYR	1024	14.949	22.909	1.953	1.00 25.94	8
ATOM	1520	C	TYR	1024	20.502	25.233	2.942	1.00 27.47	6
ATOM	1521	0	TYR	1024	19.712	25.368	3.873	1.00 27.47	8
ATOM	1522	N	GLY	1025	21.419	24.273	2.917	1.00 24.43	7
ATOM	1523	CA	GLY	1025	21.505	23.344	4.025	1.00 24.43	6
ATOM	1524	C	GLY	1025	21.593	24.073	5.356	1.00 24.43	6
ATOM	1525	ō	GLY	1025	21.032	23.619	6.356	1.00 24.43	8
ATOM	1526	N	VAL	1026	22.307	25.195	5.384	1.00 31.88	7
ATOM	1527	CA	VAL	1026	22.417	25.947	6.632	1.00 31.88	6
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ATOM	1528	CB	VAL	1026	23.566	26.979	6.609	1.00	14.56	6
ATOM	1529	CG1	VAL	1026	23.783	27.551	8.015	1.00	14.56	6
ATOM	1530	CG2	VAL	1026	24.835	26.301	6.132	1.00	14.56	6
ATOM	1531	С	VAL	1026	21.077	26.636	6.908		31.88	6
ATOM	1532	0	VAL	1026	20.691	26.833	8.062	1.00		8
ATOM	1533	N	LEU	1027	20.348	26.978	5.855		36.84	7
ATOM	1534	CA	LEU	1027	19.063	27.591	6.078	1.00	36.84	6
ATOM	1535	CB	LEU	1027	18.470	28.110	4.777			
ATOM	1536	CG	LEU	1027	17.030	28.620		1.00	5.00	6
ATOM	1537		LEU	1027			4.806	1.00	5.00	6
ATOM	1538		LEU		16.683	29.318	6.095	1.00	5.00	6
ATOM				1027	16.893	29.549	3.640	1.00	5.00	6
ATOM	1539 1540	C	LEU	1027	18.149	26.556	6.711	1.00	36.84	6
			LEU	1027	17.383	26.885	7.606	1.00	36.84	8
ATOM	1541	N	LEU	1028	18.234	25.304	6.272	1.00	19.77	7
ATOM	1542	CA	LEU	1028	17.390	24.264	6.848	1.00	19.77	6
ATOM	1543	CB	LEU	1028	17.645	22.931	6.147	1.00	24.80	6
MOTA	1544	CG	LEU	1028	16.802	21.696	6.487	1.00	24.80	6
MOTA	1545		LEU	1028	15.298	21.976	6.507	1.00	24.80	6
MOTA	1546		LEU	1028	17.117	20.681	5.417	1.00	24.80	6
ATOM	1547	C	LEU	1028	17.681	24.145	8.339	1.00	19.77	6
ATOM	1548	0	LEU	1028	16.779	23.912	9.136	1.00	19.77	8
ATOM	1549	N	TRP	1029	18.944	24.309	8.714		26.73	7
ATOM	1550	CA	TRP	1029	19.318	24.241	10.114		26.73	6
ATOM	1551	CB	TRP	1029	20.836	24.229	10.257		36.84	6
ATOM	1552	CG	TRP	1029	21.363	24.082	11.678		36.84	6
ATOM	1553	CD2	TRP	1029	21.634	25.145	12.611		36.84	6
ATOM	1554	CE2	TRP	1029	22.215	24.556	13.757		36.84	6
ATOM	1555	CE3	TRP	1029	21.438	26.536	12.588		36.84	6
ATOM	1556		TRP	1029	21.774	22.926	12.292		36.84	6
ATOM	1557		TRP	1029	22.292	23.202	13.539		36.84	7
ATOM	1558	CZ2		1029	22.613	25.310	14.860		36.84	6
ATOM	1559		TRP	1029	21.830	27.283	13.682		36.84	6
ATOM	1560		TRP	1029	22.409	26.670	14.803		36.84	6
ATOM	1561	C	TRP	1029	18.736	25.435				
ATOM	1562	ō	TRP	1029	18.498	25.314	10.898	1.00		6
ATOM	1563	N	GLU	1030					26.73	8
ATOM	1564	CA	GLU	1030	18.520	26.590	10.266	1.00	28.62	7
ATOM	1565	CB	GLU		17.958	27.734	10.996	1.00		6
ATOM	1566	CG		1030	18.082	29.020	10.177		33.13	6
ATOM	1567	CD	GLU	1030	19.486	29.535	10.077		33.13	6
ATOM			GLU	1030	19.635	30.718	9.135	1.00	33.13	6
	1568		GLU	1030	19.628	30.498	7.909	1.00	33.13	8
ATOM	1569	OE2	GLU	1030	19.756	31.865	9.625	1.00	33.13	8
ATOM	1570	C	GLU	1030	16.494	27.467	11.333	1.00	28.62	6
ATOM	1571	0	GLU	1030	16.066	27.619	12.470	1.00	28.62	8
ATOM	1572	N	ILE	1031	15.746	27.065	10.314	1.00	23.86	7
ATOM	1573	CA	ILE	1031	14.328	26.733	10.413	1.00	23.86	6
ATOM	1574	CB	ILE	1031	13.845	26.094	9.083	1.00	5.00	6
ATOM	1575		ILE	1031	12.626	25.263	9.308	1.00	5.00	6
ATOM	1576		ILE	1031	13.660	27.181	8.029	1.00	5.00	6
ATOM	1577		ILE	1031	13.157	26.703	6.709	1.00	5.00	6
ATOM	1578	C	ILE	1031	14.085	25.760	11.544	1.00	23.86	6
MOTA	1579	0	ILE	1031	13.202	25.946	12.357	1.00	23.86	8
ATOM	1580	N	VAL	1032	14.894	24.723	11.595	1.00	16.66	7
ATOM	1581	CA	VAL	1032	14.745	23.717	12.611	1.00	16.66	6
ATOM	1582	CB	VAL	1032	15.538	22.452	12.184	1.00	12.88	6
ATOM	1583	CG1	VAL	1032	15.873	21.594	13.367	1.00	12.88	6
ATOM	1584	CG2	VAL	1032	14.713	21.662	11.163	1.00	12.88	6
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ATOM	1585	С	VAL	1032	15.155	24.252	13.977	1.00 16.	66 6
ATOM	1586	ō	VAL	1032	14.456	24.032	14.952	1.00 16.	
ATOM	1587	N	SER	1033	16.258	24.986	14.058	1.00 33.	
ATOM	1588	CA	SER	1033	16.732	25.551	15.331	1.00 33.	
ATOM	1589	CB	SER	1033	18,173	25.982	15.197	1.00 27.	
ATOM	1590	OG	SER	1033	18.203	27.172	14.452	1.00 27.	
ATOM	1591	C	SER	1033	15.937	26.791	15.793	1.00 27.	
ATOM	1592	0	SER	1033					
ATOM	1593	N	LEU	1033	16.275 14.913	27.415 27.165	16.801 15.035	1.00 33.	
ATOM	1593	CA	LEU	1034					
ATOM	1595	CB	LEU		14.075	28.313	15.353	1.00 25.	
ATOM	1595	CG	LEU	1034	13.382	28.107	16.707	1.00 16.	
ATOM	1596		LEU		12.545	26.834	16.882	1.00 16.	
	1597		LEU	1034	11.931	26.831	18.286	1.00 16.	
ATOM ATOM	1599	CD2		1034	11.456	26.758	15.839	1.00 16.	
ATOM	1600	0	LEU	1034	14.777	29.676	15.328	1.00 25.	
ATOM	1601	N	LEU	1034	14.641	30.476	16.254	1.00 25.	
			GLY	1035	15.519	29.927	14.256	1.00 32.	
ATOM	1602	CA	GLY	1035	16.185	31.202	14.092	1.00 32.	
ATOM ATOM	1603	C	GLY	1035	17.458	31.404	14.866	1.00 32.	
ATOM	1604 1605	N	GLY	1035 1036	17.832	32.537	15.149 15.224	1.00 32.	
ATOM	1605	CA	GLY		18.124	30.316			
ATOM	1607	C	GLY	1036 1036	19.371 20.486	30.430	15.957 14.974	1.00 12.	
ATOM	1608	0	GLY	1036					
ATOM	1609	N	THR	1036	20.355	30.393	13.789		
ATOM	1610	CA	THR	1037	21.572 22.712	31.293	15.457 14.609	1.00 38.	
ATOM	1611	CB	THR	1037	23.593	31.608	15.266	1.00 38.	
ATOM	1612		THR	1037	22.813	33.907	15.442	1.00 32.	
ATOM	1613		THR	1037	24.754	33.907	14.387	1.00 32.	
ATOM	1614	C	THR	1037	23.519	30.323	14.418	1.00 32.	
ATOM	1615	ō	THR	1037	23.687	29.555	15.359	1.00 38.	
ATOM	1616	N	PRO	1038	24.003	30.054	13.193	1.00 51.	
ATOM	1617	CD	PRO	1038	23.734	30.837	11.973	1.00 42.	
ATOM	1618	CA	PRO	1038	24.791	28.859	12.863	1.00 51.	
ATOM	1619	CB	PRO	1038	24.677	28.776	11.354	1.00 42.	
ATOM	1620	CG	PRO	1038	24.691	30.218	10.977	1.00 42.	
ATOM	1621	С	PRO	1038	26.233	28.968	13.308	1.00 51.	
ATOM	1622	ō	PRO	1038	26.873	30.002	13.113	1.00 51.	
ATOM	1623	N	TYR	1039	26.753	27.895	13.886	1.00 44.	
ATOM	1624	CA	TYR	1039	28.124	27.909	14.349	1.00 44.	
ATOM	1625	CB	TYR	1039	29.082	28.341	13.221	1.00 38.	
ATOM	1626	CG	TYR	1039	28.980	27.544	11.933	1.00 38.	
ATOM	1627	CD1	TYR	1039	28.593	28.161	10.739	1.00 38.	
ATOM	1628	CE1	TYR	1039	28.487	27.434	9.545	1.00 38.	97 6
ATOM	1629	CD2	TYR	1039	29.263	26.185	11.907	1.00 38.	
ATOM	1630	CE2	TYR	1039	29.165	25.455	10.730	1.00 38.	97 6
ATOM	1631	CZ	TYR	1039	28.773	26.082	9.553	1.00 38.	97 6
ATOM	1632	OH	TYR	1039	28.647	25.353	8.396	1.00 38.	97 8
ATOM	1633	C	TYR	1039	28.176	28.932	15.479	1.00 44.	91 6
ATOM	1634	0	TYR	1039	29.152	29.674	15.601	1.00 44.	91 8
ATOM	1635	N	CYS	1040	27.120	28.989	16.293	1.00 52.	33 7
ATOM	1636	CA	CYS	1040	27.093	29.933	17.411	1.00 52.	
ATOM	1637	CB	CYS	1040	25.700	30.015	18.046	1.00 51.	31 6
ATOM	1638	SG	CYS	1040	25.484	31.409	19.213	1.00 51.	
ATOM	1639	C	CYS	1040	28.094	29.416	18.424	1.00 52.	
ATOM	1640	0	CYS	1040	28.113	28.224	18.729	1.00 52.	
ATOM	1641	N	GLY	1041	28.930	30.315	18.928	1.00 33.	04 7

Inventors:

Nancy J. Bump etal.

ATOM	1642	CA	GLY	1041	29.930	29.917	19.895	1.00 33.04	6
ATOM	1643	C	GLY	1041	31.293	29.745	19.257	1.00 33.04	6
ATOM	1644	0	GLY	1041	32,207	29.176	19.855	1.00 33.04	8
ATOM	1645	N	MET	1042	31.435	30.206	18.024	1.00 54.51	7
ATOM	1646	CA	MET	1042	32.718	30.129	17.350	1.00 54.51	6
		CB	MET	1042	32.713	29.085	16.241	1.00 40.53	6
ATOM	1647							1.00 40.53	6
ATOM	1648	CG	MET	1042	33.032	27.691	16.710		
ATOM	1649	SD	MET	1042	32.920	26.501	15.349	1.00 40.53	16
MOTA	1650	CE	MET	1042	31.539	25.362	15.966	1.00 40.53	6
ATOM	1651	C	MET	1042	33.029	31.492	16.785	1.00 54.51	6
MOTA	1652	0	MET	1042	32.195	32.395	16.804	1.00 54.51	8
ATOM	1653	N	THR	1043	34.241	31.633	16.286	1.00 54.86	7
ATOM	1654	CA	THR	1043	34.677	32.894	15.726	1.00 54.86	6
ATOM	1655	CB	THR	1043	36.055	33.252	16.229	1.00 82.76	6
ATOM	1656	OG1	THR	1043	36.987	32.269	15.763	1.00 82.76	8
ATOM	1657	CG2	THR	1043	36.069	33.282	17.735	1.00 82.76	6
ATOM	1658	С	THR	1043	34.780	32.796	14.227	1.00 54.86	6
ATOM	1659	ō	THR	1043	34.695	31.710	13.659	1.00 54.86	8
ATOM	1660	N	CYS	1044	35.002	33.943	13.599	1.00 95.17	7
ATOM	1661	CA	CYS	1044	35.142	34.000	12.158	1.00 95.17	6
							11.692	1.00 93.17	6
ATOM	1662	CB	CYS	1044	35.205 33.676	35.453 36.379	11.852	1.00 93.17	16
ATOM	1663	SG	CYS	1044				1.00 95.17	6
MOTA	1664	C	CYS	1044	36.396	33.272	11.681		
ATOM	1665	0	CYS	1044	36.622	33.174	10.483	1.00 95.17	8
ATOM	1666	N	ALA	1045	37.215	32.773	12.603	1.00 38.28	7
ATOM	1667	CA	ALA	1045	38.428	32.079	12.197	1.00 38.28	6
ATOM	1668	CB	ALA	1045	39.618	32.633	12.941	1.00 50.33	6
ATOM	1669	C	ALA	1045	38.348	30.571	12.387	1.00 38.28	6
ATOM	1670	0	ALA	1045	38.780	29.817	11.517	1.00 38.28	8
ATOM	1671	N	GLU	1046	37.822	30.131	13.526	1.00 39.84	7
ATOM	1672	CA	GLU	1046	37.712	28.702	13.787	1.00 39.84	6
ATOM	1673	CB	GLU	1046	36.911	28.460	15.068	1.00 83.44	6
ATOM	1674	CG	GLU	1046	37.622	28.995	16.300	1.00 83.44	6
ATOM	1675	CD	GLU	1046	36.997	28.556	17.607	1.00 83.44	6
ATOM	1676		GLU	1046	36.872	27.334	17.835	1.00 83.44	8
ATOM	1677		GLU	1046	36.635	29.442	18.408	1.00 83.44	8
ATOM	1678	C	GLU	1046	37.051	28.027	12.591	1.00 39.84	6
ATOM	1679	ō	GLU	1046	37.370	26.884	12.245	1.00 39.84	8
ATOM	1680	N	LEU	1047	36.148	28.772	11.953	1.00 55.18	7
		CA				28.312	10.771	1.00 55.18	6
ATOM	1681		LEU	1047	35.412 34.315	29.312	10.771	1.00 58.88	6
ATOM	1682	CB	LEU	1047					6
MOTA	1683	CG	LEU	1047	33.325	29.563	11.565	1.00 58.88	
ATOM	1684		LEU	1047	32.333	30.619	11.148	1.00 58.88	6
MOTA	1685		LEU	1047	32.610	28.260	11.906	1.00 58.88	6
MOTA	1686	C	LEU	1047	36.307	28.092	9.548	1.00 55.18	6
ATOM	1687	0	LEU	1047	36.106	27.157	8.786	1.00 55.18	8
ATOM	1688	N	TYR	1048	37.283	28.967	9.352	1.00 49.08	7
ATOM	1689	CA	TYR	1048	38.203	28.820	8.234	1.00 49.08	6
ATOM	1690	CB	TYR	1048	39.033	30.097	8.078	1.00 62.53	6
ATOM	1691	CG	TYR	1048	38.422	31.088	7.123	1.00 62.53	6
ATOM	1692		TYR	1048	37.554	32.092	7.559	1.00 62.53	6
ATOM	1693		TYR	1048	36.956	32.963	6.644	1.00 62.53	6
ATOM	1694		TYR	1048	38.678	30.981	5.765	1.00 62.53	6
ATOM	1695	CE2		1048	38.096	31.829	4.851	1.00 62.53	6
ATOM	1696	CZ	TYR	1048	37.233	32.820	5.280	1.00 62.53	6
ATOM	1697	OH	TYR	1048	36.649	33.642	4.333	1.00 62.53	8
ATOM	1698	C	TYR	1048		27.618	8.525	1.00 49.08	6
ALUM	1020	_	TIK	1040	39.112	27.010	0.525	2.00 45.00	

ATOM	1699	0	TYR	1048	39.661	27.008	7.603	1.00 49.08	8
ATOM	1700	N	GLU	1049	39.224	27.293	9.817	1.00 50.97	7
ATOM	1701	CA	GLU	1049	40.047	26.196	10.341	1.00 50.97	6
ATOM	1702	CB	GLU	1049	40.532	26.543	11.761	1.00 95.40	6
ATOM	1703	CG	GLU	1049	41.455	25.483	12.408	1.00 95.40	6
ATOM	1704	CD	GLU	1049	41.583	25.610	13.940	1.00 95.40	6
ATOM	1705		GLU	1049	41.872	26.717	14.445	1.00 95.40	8
ATOM	1706	OE2	GLU	1049	41.397	24.589	14.641	1.00 95.40	8
ATOM	1707	C	GLU	1049	39.347	24.829	10.395	1.00 50.97	6
ATOM	1708	ō	GLU	1049	39.581	23.962	9.543	1.00 50.97	8
ATOM	1709	N	LYS	1050	38.499	24.659	11.416	1.00 80.24	7
ATOM	1710	CA	LYS	1050	37.750	23.420	11.683	1.00 80.24	6
ATOM	1711	CB	LYS	1050	37.730	23.446	13.105	1.00 32.58	6
ATOM	1712	C	LYS	1050	36.603	23.121	10.729	1.00 80.24	6
ATOM	1713	0	LYS	1050	35.910	22.112	10.729	1.00 80.24	8
	1714	N				23.993	9.757	1.00 50.24	7
ATOM			LEU	1051	36.394	23.769	8.810	1.00 50.22	6
ATOM	1715	CA	LEU	1051	35.323	25.081	8.449	1.00 30.22	6
ATOM	1716	CB	LEU	1051	34.627		7.780	1.00 21.77	6
ATOM	1717	CG	LEU	1051	33.258	24.954			6
ATOM	1718		LEU	1051	32.248	24.632	8.834	1.00 21.77	6
ATOM	1719		LEU	1051	32.900	26.226	7.065	1.00 21.77	6
ATOM	1720	C	LEU	1051	35.827	23.121	7.540	1.00 50.22	
ATOM	1721	0	TEU	1051	35.308	22.098	7.123	1.00 50.22	8
ATOM	1722	N	PRO	1052	36.860	23.692	6.913	1.00 73.14	7
ATOM	1723	CD	PRO	1052	37.819	24.695	7.400	1.00 57.36	6
ATOM	1724	CA	PRO	1052	37.372	23.122	5.675	1.00 73.14	6
ATOM	1725	CB	PRO	1052	38.669	23.898	5.460	1.00 57.36	6
ATOM	1726	CG	PRO	1052	38.368	25.214	6.097	1.00 57.36	6
ATOM	1727	С	PRO	1052	37.600	21.638	5.814	1.00 73.14	6
ATOM	1728	0	PRO	1052	36.747	20.823	5.474	1.00 73.14	8
ATOM	1729	N	GLN	1053	38.756	21.308	6.359	1.00 77.10	7
ATOM	1730	CA	GLN	1053	39.139	19.932	6.542	1.00 77.10	6
ATOM	1731	CB	GLN	1053	40.574	19.886	7.003	1.00100.00	6
MOTA	1732	С	GLN	1053	38.256	19.137	7.504	1.00 77.10	6
ATOM	1733	0	GLN	1053	38.279	17.904	7.479	1.00 77.10	8
ATOM	1734	N	GLY	1054	37.475	19.815	8.341	1.00 78.88	7
ATOM	1735	CA	GLY	1054	36.658	19.075	9.293	1.00 78.88	6
ATOM	1736	C	GLY	1054	35.160	18.960	9.074	1.00 78.88	6
ATOM	1737	0	GLY	1054	34.644	19.099	7.965	1.00 78.88	8
ATOM	1738	N	TYR	1055	34.460	18.683	10.164	1.00 61.80	7
ATOM	1739	CA	TYR	1055	33.018	18.525	10.146	1.00 61.80	6
ATOM	1740	CB	TYR	1055	32.547	17.902	11.458	1.00100.00	6
ATOM	1741	CG	TYR	1055	32.642	18.897	12.598	1.00100.00	6
ATOM	1742		TYR	1055	31.499	19.464	13.161	1.00100.00	6
ATOM	1743	CE1	TYR	1055	31.592	20.444	14.144	1.00100.00	6
ATOM	1744	CD2	TYR	1055	33.885	19.337	13.057	1.00100.00	6
ATOM	1745	CE2	TYR	1055	33.985	20.316	14.039	1.00100.00	6
ATOM	1746	CZ	TYR	1055	32.835	20.860	14.571	1.00100.00	6
ATOM	1747	OH	TYR	1055	32.928	21.827	15.531	1.00100.00	8
ATOM	1748	С	TYR	1055	32.344	19.891	10.001	1.00 61.80	6
ATOM	1749	0	TYR	1055	32.982	20.912	9.728	1.00 61.80	8
ATOM	1750	N	ARG	1056	31.038	19.885	10.231	1.00 78.80	7
ATOM	1751	CA	ARG	1056	30.216	21.079	10.155	1.00 78.80	6
ATOM	1752	CB	ARG	1056	29.674	21.216	8.729	1.00 56.27	6
MOTA	1753	CG	ARG	1056	29.456	19.890	8.001	1.00 56.27	6
ATOM	1754	CD	ARG	1056	29.992	19.943	6.563	1.00 56.27	6
ATOM	1755	NE	ARG	1056	31.444	19.832	6.494	1.00 56.27	7

FIG. 3EE

Inventors: Nancy J. Bump et al.

| 1756 | C2 | ARG | 1056 | 32.115 | 19.413 | 5.425 | 1.00 | 56.27 | 1758 | NH1 | ARG | 1056 | 31.468 | 19.062 | 4.323 | 1.00 | 56.27 | 1758 | NH2 | ARG | 1056 | 29.074 | 21.074 | 11.192 | 1.00 | 78.80 | 1756 | 29.074 | 21.074 | 11.192 | 1.00 | 78.80 | 1760 | 0 | ARG | 1056 | 29.074 | 21.074 | 11.192 | 1.00 | 78.80 | 1761 | N | LEU | 1057 | 28.149 | 22.030 | 11.081 | 1.00 | 52.45 | 1762 | CA | LEU | 1057 | 25.915 | 23.018 | 11.375 | 1.00 | 37.29 | 1763 | CB | LEU | 1057 | 25.915 | 23.018 | 11.375 | 1.00 | 37.29 | 1766 | CD1 | LEU | 1057 | 25.208 | 25.439 | 10.966 | 1.00 | 37.29 | 1766 | CD2 | LEU | 1057 | 26.208 | 25.439 | 10.966 | 1.00 | 37.29 | 1766 | CD2 | LEU | 1057 | 26.208 | 25.439 | 10.966 | 1.00 | 37.29 | 1766 | CD2 | LEU | 1057 | 26.208 | 25.439 | 10.966 | 1.00 | 37.29 | 1766 | CD2 | LEU | 1057 | 26.208 | 25.439 | 10.966 | 1.00 | 37.29 | 1766 | CD2 | LEU | 1057 | 26.208 | 25.439 | 10.966 | 1.00 | 37.29 | 1766 | CD2 | LEU | 1057 | 26.208 | 25.439 | 10.966 | 1.00 | 37.29 | 1766 | CD2 | LEU | 1057 | 26.208 | 25.439 | 10.966 | 1.00 | 37.29 | 1767 | CA | GLU | 1058 | 26.264 | 20.978 | 13.955 | 1.00 | 52.45 | 1770 | CA | GLU | 1058 | 25.730 | 19.856 | 14.739 | 1.00 | 65.26 | 1771 | CB | GLU | 1058 | 25.6264 | 20.978 | 13.955 | 1.00 | 65.26 | 1772 | CG | GLU | 1058 | 25.940 | 21.232 | 16.943 | 1.00 | 73.19 | 1773 | CD | GLU | 1058 | 26.617 | 22.450 | 16.375 | 1.00 | 73.19 | 1775 | OE2 | GLU | 1058 | 26.617 | 22.450 | 16.375 | 1.00 | 73.19 | 1775 | OE2 | GLU | 1058 | 26.158 | 23.611 | 16.679 | 1.00 | 73.19 | 1776 | CB | GLU | 1058 | 26.158 | 23.611 | 16.679 | 1.00 | 73.19 | 1776 | CB | LU | 1058 | 26.251 | 19.40 | 16.1375 | 1.00 | 63.67 | 1779 | CA | LYS | 1059 | 22.222 | 18.230 | 14.756 | 1.00 | 63.67 | 1779 | CA | LYS | 1059 | 22.222 | 18.230 | 14.756 | 1.00 | 63.67 | 1782 | CD | LYS | 1059 | 22.222 | 18.230 | 14.756 | 1.00 | 63.67 | 1782 | CD | LYS | 1059 | 20.066 | 15.034 | 14.104 | 1.00 | 63.67 | 1782 | CD | LYS | 1059 | 20.066 | 15.034 | 14.104 | 1.00 | 63.67 | 1786 | CD | LYS | 1059 | 20.066 | 15.034 | 1 ATOM 1756 CZ ARG 1056 32.115 19.413 5.425 1.00 56.27 ATOM MOTA ATOM ATOM ATOM ATOM ATOM ATOM 17.476 19.851 21.443 1.00 82.15 18.413 20.859 20.777 1.00 82.15 16.033 20.116 21.048 1.00 82.15 16.562 17.680 19.047 1.00 79.51 16.187 16.513 19.026 1.00 79.51 15.802 18.696 18.631 1.00 43.98 14.437 18.512 18.124 1.00 43.98 13.689 19.843 18.124 1.00 26.42 ATOM ATOM ATOM 1800 C LEU 1061 ATOM 1802 N ASN 1062 15.802 18.696 18.631 1.00 43.98
ATOM 1803 CA ASN 1062 13.689 19.843 18.124 1.00 26.42
ATOM 1804 CB ASN 1062 13.689 19.843 18.124 1.00 26.42
ATOM 1805 CG ASN 1062 13.689 19.843 18.124 1.00 26.42
ATOM 1806 OD1 ASN 1062 15.554 21.327 17.834 1.00 26.42
ATOM 1807 ND2 ASN 1062 15.554 21.327 17.834 1.00 26.42
ATOM 1808 C ASN 1062 15.958 21.430 16.294 1.00 26.42
ATOM 1808 C ASN 1062 13.908 21.430 16.294 1.00 26.42
ATOM 1809 O ASN 1062 13.908 21.430 16.294 1.00 26.42
ATOM 1809 O ASN 1062 13.908 21.430 16.594 1.00 43.98
ATOM 1810 N CYS 1063 15.646 17.914 16.143 1.00 43.98
ATOM 1811 CA CYS 1063 15.767 17.460 14.769 1.00 48.23
ATOM 1812 CB CYS 1063 16.914 18.199 14.103 1.00 48.23 MOTA 1801 O LEU 1061

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FIG. 3FF

ATOM	1813	SG	CYS	1063	16.932	17.981	12.363	1.00 49.76	16
ATOM	1814	C	CYS	1063	15.943	15.948	14.559	1.00 48.23	6
ATOM	1815	0	CYS	1063	16.912	15.361	15.039	1.00 48.23	8
ATOM	1816	N	ASP	1064	15.001	15.338	13.834	1.00 41.84	7
ATOM	1817	CA	ASP	1064	15.029	13.907	13.522	1.00 41.84	6
ATOM	1818	CB	ASP	1064	13.788	13.487	12.715	1.00 55.35	6
ATOM	1819	CG	ASP	1064	13.829	12.012	12.290	1.00 55.35	6
MOTA	1820		ASP	1064	13.977	11.154	13.175	1.00 55.35	8
ATOM	1821	OD2	ASP	1064	13.712	11.710	11.086	1.00 55.35	8
ATOM	1822	С	ASP	1064	16.273	13.599	12.702	1.00 41.84	6
ATOM	1823	0	ASP	1064	16.918	14.521	12.181	1.00 41.84	8
ATOM	1824	N	ASP	1065	16.602	12.309	12.576	1.00 68.56	7
MOTA	1825	CA	ASP	1065	17.789	11.871	11.825	1.00 68.56	6
MOTA	1826	CB	ASP	1065	 18.094	10.391	12.086	1.00100.00	6
MOTA	1827	CG	ASP	1065	18.357	10.088	13.549	1.00100.00	6
ATOM	1828		ASP	1065	17.400	10.124	14.341	1.00100.00	8
ATOM	1829		ASP	1065	19.524	9.820	13.894	1.00100.00	8
ATOM	1830	C	ASP	1065	17.654	12.072	10.321	1.00 68.56	6
ATOM	1831	0	ASP	1065	18.627	12.404	9.644	1.00 68.56	8
ATOM	1832	N	GLU	1066	16.457	11.850	9.797	1.00 54.29	7
ATOM	1833	CA	GLU	1066	16.247	12.025	8.378	1.00 54.29	6
ATOM	1834	CB	GLU	1066	14.843	11.583	8.001	1.00 91.86	6
ATOM	1835	CG	GLU	1066	14.550	10.152	8.383	1.00 91.86	6
ATOM	1836	CD	GLU	1066	13.252	9.651	7.787	1.00 91.86	6
ATOM	1837		GLU	1066	12.729	8.615	8.258	1.00 91.86	8
ATOM	1838		GLU	1066	12.755	10.296	6.840	1.00 91.86	8
ATOM	1839	C	GLU	1066	16.481	13.479	7.989	1.00 54.29	6
MOTA	1840	0	GLU	1066	17.223	13.758	7.048	1.00 54.29	8
ATOM	1841	N	VAL	1067	15.878	14.408	8.727	1.00 46.62	7
MOTA	1842	CA	VAL	1067	16.032	15.836	8.426	1.00 46.62	6
MOTA	1843	CB	VAL	1067	15.277	16.712	9.430	1.00 20.69	6
MOTA	1844		VAL	1067	15.286	18.154	8.957	1.00 20.69	6
ATOM	1845		VAL	1067	13.879	16.208	9.595	1.00 20.69	6
ATOM	1846	C	VAL	1067	17.484	16.314	8.400	1.00 46.62	6
ATOM	1847	0	VAL	1067	17.892	17.076	7.526	1.00 46.62	8
ATOM	1848	N	TYR	1068	18.261	15.858	9.367	1.00 49.64	7
MOTA	1849	CA	TYR	1068	19.654	16.240	9.459	1.00 49.64	6
ATOM	1850	CB	TYR	1068	20.195	15.811	10.813	1.00 42.96	6
MOTA	1851	CG	TYR	1068	21.604	16.239	11.074	1.00 42.96	6
ATOM ATOM	1852 1853	CE1	TYR	1068	21.947	17.594	11.093 11.387	1.00 42.96	6
ATOM	1854	CD2	TYR	1068	23.236	18.006 15.301	11.387	1.00 42.96	6
ATOM	1855	CE2							6
ATOM	1856	CZ	TYR	1068	23.882	15.701	11.640 11.662	1.00 42.96	6
ATOM	1857	OH	TYR	1068	24.198	17.055 17.451	11.002	1.00 42.96	8
ATOM	1858	C	TYR	1068	20.424	15.557	8.338	1.00 42.98	6
ATOM	1859	0	TYR	1068	21.239	16.176	7.663	1.00 49.64	8
ATOM	1860	N	ASP	1069	20.148	14.275	8.144	1.00 54.25	7
ATOM	1861	CA	ASP	1069		13.495	7.112	1.00 54.25	6
ATOM	1862	CB	ASP	1069	20.808	12.188	6.905	1.00100.00	6
ATOM	1863	CG	ASP	1069	20.812	11.231	6.043	1.00100.00	6
ATOM	1864		ASP	1069	21.225	11.635	4.937	1.00100.00	8
ATOM	1865		ASP	1069	20.986	10.076	6.479	1.00100.00	8
ATOM	1866	C	ASP	1069	20.986	14.279	5.803	1.00100.00	6
ATOM	1867	0	ASP	1069	21.779	14.219	5.037	1.00 54.25	8
ATOM	1868	N	LEU	1070	19.697	14.247	5.562	1.00 40.31	7
ATOM	1869	CA	LEU	1070	19.496	15.777	4.371	1.00 40.31	6
PER OPT	2009	~~	1110	10,0	20.200	20.777	4.5/1	2.00 40.31	_

ATOM	1870	CB	LEU	1070	18.009	16.075	4.195	1.00 25.05	6
ATOM	1871	CG	LEU	1070	17.581	16.966	3.048	1.00 25.05	6
ATOM	1872	CD1	LEU	1070	17.865	16.291	1.720	1.00 25.05	6
ATOM	1873		LEU	1070	16.114	17.219	3.219	1.00 25.05	6
ATOM	1874	C	LEU	1070	20.290	17.079	4.447	1.00 40.31	6
ATOM	1875	0	LEU	1070	20.561	17.688	3.423	1.00 40.31	8
ATOM	1876	N	MET	1071	20.639	17.510	5.655	1.00 23.05	7
ATOM	1877	CA	MET	1071	21.452	18.703	5.785	1.00 23.05	6
ATOM	1878	CB	MET	1071	21.367	19.310	7.201	1.00 19.93	6
ATOM	1879	CG	MET	1071	20.030	19.910	7.631	1.00 19.93	6
ATOM	1880	SD	MET	1071	20.077	20.344	9.411	1.00 19.93	16
ATOM	1881	CE	MET	1071	18.390	20.649	9.751	1.00 19.93	6
ATOM	1882	C	MET	1071	22.888	18.243	5.504	1.00 23.05	6
ATOM	1883	0	MET	1071	 23.591	18.880	4.744	1.00 23.05	8
ATOM	1884	N	ARG	1072	23.319	17.124	6.082	1.00 51.65	7
ATOM	1885	CA	ARG	1072	24.689	16.669	5.864	1.00 51.65	6
ATOM	1886	CB	ARG	1072	24.978	15.434	6.696	1.00 98.84	6
ATOM	1887	CG	ARG	1072	24.870	15.716	8.162	1.00 98.84	6
ATOM	1888	CD	ARG	1072	26.125	16.339	8.727	1.00 98.84	6
ATOM	1889	NE	ARG	1072	27.004	15.305	9.271	1.00 98.84	7
ATOM	1890	CZ	ARG	1072	27.992	15.530	10.131	1.00 98.84	6
ATOM	1891	NH1	ARG	1072	28.232	16.767	10.546	1.00 98.84	7
ATOM	1892	NH2	ARG	1072	28.724	14.521	10.593	1.00 98.84	7
ATOM	1893	C	ARG	1072	25.023	16.404	4.401	1.00 51.65	6
ATOM	1894	0	ARG	1072	26.150	16.659	3.973	1.00 51.65	8
ATOM	1895	N	GLN	1073	24.073	15.900	3.617	1.00 27.54	7
ATOM	1896	CA	GLN	1073	24.376	15.679	2.211	1.00 27.54	6
ATOM	1897	CB	GLN	1073	23.347	14.746	1.568	1.00 67.93	6
ATOM	1898	CG	GLN	1073	21.934	15.149	1.789	1.00 67.93	6
ATOM	1899	CD	GLN	1073	20.972	14.026	1.527	1.00 67.93	6
ATOM	1900		GLN	1073	20.889	13.066	2.298	1.00 67.93	8
ATOM	1901	NE2		1073	20.238	14.127	0.422	1.00 67.93	7
ATOM	1902	C	GLN	1073	24.449	17.041	1.500	1.00 27.54	6
MOTA	1903	0	GLN	1073	25.088	17.162	0.453	1.00 27.54	8
ATOM	1904	N	CYS	1074	23.816	18.070	2.072	1.00 36.16	7
MOTA	1905	CA	CYS	1074	23.858	19.423	1.497	1.00 36.16	6
ATOM	1906	CB	CYS	1074	22.925	20.393	2.243	1.00 40.38	6
ATOM	1907	SG	CYS	1074	21.201	20.463	1.797	1.00 40.38	16
ATOM	1908	С	CYS	1074	25.282	19.995	1.627	1.00 36.16	6
ATOM	1909	0	CYS	1074	25.746	20.748	0.767	1.00 36.16	8
ATOM	1910	N	TRP	1075	25.958	19.619	2.716	1.00 26.48	7
ATOM	1911	CA	TRP	1075	27.302	20.120	3.049	1.00 26.48	6
ATOM	1912	CB	TRP	1075	27.413	20.389	4.570	1.00 32.15	6
ATOM	1913	CG	TRP	1075	26.260	21.224	5.181	1.00 32.15	6
ATOM	1914	CD2	TRP	1075	25.679	21.080	6.485	1.00 32.15	6
ATOM	1915	CE2	TRP	1075	24.682	22.075	6.613	1.00 32.15	6
ATOM	1916	CE3	TRP	1075	25.901	20.211	7.553	1.00 32.15	6
MOTA	1917	CD1	TRP	1075	25.607	22.272	4.597	1.00 32.15	6
ATOM	1918	NE1	TRP	1075	24.662	22.783	5.449	1.00 32.15	7
ATOM	1919	CZ2	TRP	1075	23.909	22.222	7.774	1.00 32.15	6
ATOM	1920	CZ3	TRP	1075	25.133	20.361	8.703	1.00 32.15	6
ATOM	1921	CH2	TRP	1075	24.148	21.357	8.807	1.00 32.15	6
ATOM	1922	C	TRP	1075	28.471	19.236	2.622	1.00 26.48	б
ATOM	1923	0	TRP	1075	29.599	19.447	3.071	1.00 26.48	8
ATOM ATOM	1924 1925	N	ARG	1076	28.209	18.265	1.751	1.00 51.58	7
ATOM		CA	ARG	1076	29.258	17.367	1.279	1.00 51.58	6
ATOM	1926	CB	ARG	1076	28.683	16.391	0.249	1.00 67.56	6

MOTA	1927	CG	ARG	1076		27.618	15.509	0.847	1.00	67.56	6
ATOM	1928	CD	ARG	1076		27.279	14.291	0.009	1.00	67.56	6
ATOM	1929	NE	ARG	1076		26.267	13.485	0.690	1.00		7
MOTA	1930	CZ	ARG	1076		25.731	12.365	0.215	1.00	67.56	6
ATOM	1931		ARG	1076		26.104	11.891	-0.966	1.00	67.56	7
ATOM	1932	NH2	ARG	1076		24.819	11.714	0.929	1.00		7
ATOM	1933	С	ARG	1076		30.431	18.157	0.710	1.00	51.58	6
ATOM	1934	0	ARG	1076		30.238	19.206	0.103	1.00	51.58	8
ATOM	1935	N	GLU	1077		31.642	17.651	0.941	1.00	50.74	7
ATOM	1936	CA	GLU	1077		32.885	18.281	0.488	1.00	50.74	6
ATOM	1937	CB	GLU	1077		34.059	17.419	0.893	1.00	91.21	6
ATOM	1938	C	GLU	1077		32.927	18.540	-1.013	1.00 !	50.74	6
ATOM	1939	0	GLU	1077		33.213	19.657	-1.450	1.00	50.74	8
ATOM	1940	N	LYS	1078	-0.0	32.656	17.494	-1.790	1.00	49.20	7
ATOM	1941	CA	LYS	1078		32.657	17.579	-3.240	1.00	49.20	6
ATOM	1942	CB	LYS	1078		32.895	16.197	-3.847	1.00	93.58	6
ATOM	1943	CG	LYS	1078		34.289	15.666	-3.640	1.00	93.51	6
ATOM	1944	CD	LYS	1078		34.458	14.341	-4.346	1.00	93.51	6
ATOM	1945	CE	LYS	1078		35.872	13.806	-4.191	1.00	93.51	6
ATOM	1946	NZ	LYS	1078		36.025	12.476	-4.860	1.00 9	93.51	7
ATOM	1947	C	LYS	1078		31.345	18.145	-3.760	1.00	49.20	6
ATOM	1948	0	LYS	1078		30.290	17.528	-3.617	1.00	49.20	8
MOTA	1949	N	PRO	1079		31.390	19.341	-4.366	1.00	30.47	7
MOTA	1950	CD	PRO	1079		32.592	20.190	-4.459	1.00 2	29.67	6
MOTA	1951	CA	PRO	1079		30.236	20.040	-4.931	1.00	30.47	6
ATOM	1952	CB	PRO	1079		30.887	21.098	-5.791	1.00	29.67	6
MOTA	1953	CG	PRO	1079		32.024	21.511	-4.914	1.00	29.67	6
MOTA	1954	C	PRO	1079		29.235	19.190	-5.711	1.00	30.47	6
MOTA	1955	0	PRO	1079		28.040	19.221	-5.420	1.00		8
ATOM	1956	N	TYR	1080		29.708	18.462	-6.718	1.00	44.53	7
ATOM	1957	CA	TYR	1080		28.821	17.616	-7.520	1.00		6
MOTA	1958	CB	TYR	1080		29.576	17.054	-8.730	1.00		6
ATOM	1959	CG	TYR	1080		30.938	16.479	-8.412	1.00		6
ATOM	1960	CD1	TYR	1080		31.072	15.207	-7.859	1.00		6
MOTA	1961	CE1	TYR	1080		32.329	14.691	-7.531	1.00		6
ATOM	1962	CD2	TYR	1080		32.095	17.223	-8.636	1.00		6
ATOM	1963	CE2	TYR	1080		33.351	16.722	-8.312	1.00		6
ATOM	1964	CZ	TYR	1080		33.462	15.458	-7.757	1.00		6
ATOM	1965	OH	TYR	1080		34.701	14.970	-7.409	1.00		8
ATOM	1966	С	TYR	1080		28.232	16.490	-6.672	1.00		6
ATOM	1967	0	TYR	1080		27.282	15.833	-7.087	1.00		8
ATOM	1968	N	GLU	1081		28.792	16.285	-5.484	1.00		7
ATOM	1969	CA	GLU	1081		28.285	15.257	-4.588	1.00		6
ATOM	1970	CB	GLU	1081		29.373	14.767	-3.638	1.00		6
ATOM	1971	CG	GLU	1081		30.292	13.713	-4.220	1.00		6
MOTA	1972	CD	GLU	1081		31.240	13.143	-3.182	1.00		6
ATOM	1973		GLU	1081		31.903	12.119	-3.470	1.00		8
MOTA	1974		GLU	1081		31.323	13.726	-2.079	1.00		8
ATOM	1975	C	GLU	1081		27.114	15.809	-3.778	1.00		6 8
ATOM	1976	0	GLU	1081		26.512	15.099	-2.972	1.00		
ATOM	1977	N	ARG	1082		26.812	17.087	-3.975	1.00		7
ATOM	1978	CA	ARG	1082		25.702	17.706	-3.280	1.00		6
ATOM	1979	CB	ARG	1082		25.979	19.207	-3.053	1.00		6
ATOM	1980	CG	ARG	1082		26.429	19.535	-1.624	1.00		6
ATOM	1981	CD	ARG	1082		27.857	20.100	-1.505	1.00		6 7
ATOM ATOM	1982	NE	ARG	1082		27.939	21.540	-1.743	1.00	30.76	6
ALOM	1983	CZ	ARG	1082		29.060	22.258	-1.663	1.00	30.76	6

ATOM	1984	MHI	ARG	1082	30.225	21.698	-1.358	1 00	30.76	7
ATOM	1985		ARG	1082	29.007	23.567	-1.865		30.76	7
ATOM	1986	C	ARG	1082	24.446	17.479	-4.124		50.75	6
ATOM	1987	ō	ARG	1082	24.501	17.497	-5.355		50.75	8
ATOM	1988	N	PRO	1083	23.303	17.225	-3.464		42.97	7
ATOM	1989	CD	PRO	1083	23.155	17.153	-1.995		16.51	6
ATOM	1990	CA	PRO	1083	22.022	16.983	-4.127		42.97	6
ATOM	1991	CB	PRO	1083	21.171	16.382	-3.015		16.51	6
ATOM	1992	CG	PRO	1083	21.665	17.079	-1.805	1.00		6
ATOM	1993	C	PRO	1083	21.450	18.268	-4.715			6
ATOM	1994	0	PRO	1083	21.430	19.353	-4.713		42.97	8
ATOM	1995	N	SER	1084	20.448	18.132	-5.564		43.29	7
ATOM	1996	CA	SER	1084	19.842	19.275	-6.217		43.29	6
ATOM	1997	CB	SER	1084	 19.553	18.890	-7.643		28.32	6
ATOM	1998	OG	SER	1084	18.965	17.607	-7.610		28.32	8
ATOM	1999	C	SER	1084	18.543	19.679	-5.538		43.29	6
ATOM	2000	0	SER	1084	17.901	18.858	-4.878		43.29	8
ATOM	2001	N	PHE	1085	18.148		-5.723			7
ATOM	2002	CA	PHE	1085	16.913	20.934	-5.128	1.00	22.83	6
ATOM	2002	CB	PHE	1085		21.427				
ATOM	2003	CG	PHE		16.688	22.881	-5.538	1.00	7.27	6
ATOM	2005	CD1		1085 1085	17.599	23.814	-4.858	1.00	7.27	6 6
ATOM	2005	CD2	PHE	1085	18.487	24.598	-5.588	1.00	7.27	
ATOM	2007		PHE	1085	17.592 19.356	23.899	-3.476 -4.949	1.00	7.27	6 6
ATOM	2007	CE2	PHE	1085	18.454	24.756	-4.949	1.00	7.27	6
ATOM	2009	CZ	PHE	1085	19.341	25.545	-3.560	1.00	7.27	6
ATOM	2010	C	PHE	1085	15.710	20.587	-5.510	1.00		6
ATOM	2011	ō	PHE	1085	14.660	20.668	-4.882	1.00	22.83	8
ATOM	2012	N	ALA	1086	15.878	19.789	-6.553		45.86	7
ATOM	2013	CA	ALA	1086	14.813	18.919	-7.016	1.00		6
ATOM	2014	CB	ALA	1086	15.037	18.540	-8.430	1.00	15.16	6
ATOM	2015	c	ALA	1086	14.783	17.674	-6.161		45.86	6
ATOM	2016	o	ALA	1086	13.720	17.175	-5.815	1.00		8
ATOM	2017	N	GLN	1087	15.959	17.180	-5.810	1.00	32.39	7
ATOM	2018	CA	GLN	1087	16.020	15.990	-5.000	1.00	32.39	6
ATOM	2019	CB	GLN	1087	17.433	15.386	-5.038		50.88	6
ATOM	2020	CG	GLN	1087	17.971	15.230	-6.466	1.00	50.88	6
ATOM	2021	CD	GLN	1087	19.290	14.488	-6.552	1.00	50.88	6
ATOM	2022	OE1	GLN	1087	20.221	14.752	-5.790	1.00	50.88	8
ATOM	2023	NE2	GLN	1087	19.389	13.577	~7.510	1.00	50.88	7
ATOM	2024	C	GLN	1087	15.617	16.398	-3.592	1.00	32.39	6
ATOM	2025	0	GLN	1087	14.792	15.737	-2.956	1.00	32.39	8
ATOM	2026	N	ILE	1088	16.177	17.507	-3.116	1.00	19.40	7
ATOM	2027	CA	ILE	1088	15.875	17.997	-1.761	1.00	19.40	6
ATOM	2028	CB	ILE	1088	16.519	19.358	-1.532	1.00	20.50	6
ATOM	2029	CG2	ILE	1088	16.172	19.905	-0.185	1.00	20.50	6
ATOM	2030		ILE	1088	18.017	19.199	-1.630	1.00	20.50	6
ATOM	2031		ILE	1088	18.747	20.459	-1.361	1.00	20.50	6
ATOM	2032	С	ILE	1088	14.375	18.102	-1.531	1.00	19.40	6
ATOM	2033	0	ILE	1088	13.852	17.646	-0.514	1.00	19.40	8
ATOM	2034	N	LEU	1089	13.697	18.700	-2.500	1.00	31.43	7
ATOM	2035	CA	LEU	1089	12.262	18.860	-2.452	1.00	31.43	6
ATOM	2036	CB	LEU	1089	11.783	19.531	-3.714	1.00	14.58	6
ATOM	2037	CG	LEU	1089	10.376	20.070	-3.576	1.00	14.58	6
ATOM	2038		LEU	1089	10.208	20.858	-2.288	1.00	14.58	6
ATOM	2039		LEU	1089	10.136	20.941	-4.788	1.00		6
ATOM	2040	С	LEU	1089	11.595	17.509	-2.335	1.00	31.43	6

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ATOM	2041	0	LEU	1089	10.804	17.270	-1.423	1.00	31.43	8
ATOM	2042	N	VAL	1090	11.920	16.619	-3.265	1.00	26.46	7
ATOM	2043	CA	VAL	1090	11.346	15.288	-3.242	1.00	26.46	6
ATOM	2044	CB	VAL	1090	12.042	14.338	-4.171	1.00	24.17	6
ATOM	2045	CG1	VAL	1090	11.419	12.957	-4.012	1.00	24.17	6
ATOM	2046	CG2	VAL	1090	11.913	14.819	-5.581	1.00	24.17	6
ATOM	2047	С	VAL	1090	11.441	14.697	-1.861	1.00	26.46	6
ATOM	2048	0	VAL	1090	10.476	14.126	-1.362		26.46	8
ATOM	2049	N	SER	1091	12.600	14.819	-1.235	1.00	24.68	7
ATOM	2050	CA	SER	1091	12.726	14.276	0.094	1.00	24.68	6
ATOM	2051	CB	SER	1091	14.156	14.407	0.599	1.00	45.28	6
ATOM	2052	OG	SER	1091	15.039	13.699	-0.249	1.00	45.28	8
ATOM	2053	C	SER	1091	11.742	14.999	1.006	1.00	24.68	6
ATOM	2054	0	SER	1091	 10.796	14.379	1.471	1.00	24.68	8
ATOM	2055	N	LEU	1092	11.919	16.302	1.231	1.00	45.44	7
ATOM	2056	CA	LEU	1092	11.001	17.031	2.112		45.44	6
ATOM	2057	CB	LEU	1092	11.127	18.557	1.905	1.00	19.86	6
ATOM	2058	CG	LEU	1092	12.518	19.144	2.242	1.00	19.86	6
ATOM	2059	CD1	LEU	1092	12.611	20.594	1.810	1.00	19.86	6
ATOM	2060	CD2	LEU	1092	12.793	19.007	3.728	1.00	19.86	6
ATOM	2061	C	LEU	1092	9.554	16.568	1.918	1.00	45.44	6
ATOM	2062	0	LEU	1092	8.821	16.438	2.891	1.00	45.44	8
ATOM	2063	N	ASN	1093	9.162	16.275	0.678	1.00	44.52	7
ATOM	2064	CA	ASN	1093	7.797	15.820	0.360		44.52	6
ATOM	2065	CB	ASN	1093	7.578	15.906	-1.147	1.00	34.39	6
ATOM	2066	CG	ASN	1093	7.266	17.302	-1.586	1.00	34.39	6
ATOM	2067	OD1	ASN	1093	7.572	17.705	-2.703	1.00	34.39	8
ATOM	2068	ND2	ASN	1093	6.639	18.061	-0.698	1.00	34.39	7
ATOM	2069	C	ASN	1093	7.501	14.414	0.849	1.00	44.52	6
ATOM	2070	0	ASN	1093	6.437	14.137	1.401	1.00	44.52	8
ATOM	2071	N	ARG	1094	8.458	13.529	0.631	1.00	42.85	7
ATOM	2072	CA	ARG	1094	8.329	12.168	1.074	1.00	42.85	6
ATOM	2073	CB	ARG	1094	9.491	11.353	0.472	1.00	83.86	6
ATOM	2074	CG	ARG	1094	10.129	10.325	1.373	1.00	83.62	6
ATOM	2075	CD	ARG	1094	11.099	10.992	2.328	1.00	83.62	6
ATOM	2076	NE	ARG	1094	11.576	10.076	3.359	1.00	83.62	7
ATOM	2077	CZ	ARG	1094	10.787	9.365	4.163	1.00	83.62	6
ATOM	2078	NHl	ARG	1094	9.466	9.461	4.070	1.00	83.62	7
ATOM	2079	NH2	ARG	1094	11.323	8.549	5.061	1.00	83.62	7
ATOM	2080	C	ARG	1094	8.293	12.166	2.628	1.00	42.85	6
ATOM	2081	0	ARG	1094	7.667	11.308	3.239	1.00	42.85	8
MOTA	2082	N	MET	1095	8.934	13.151	3.253	1.00	51.73	7
ATOM	2083	CA	MET	1095	8.991	13.279	4.712	1.00	51.73	6
ATOM	2084	CB	MET	1095	10.206	14.135	5.109	1.00	28.03	6
ATOM	2085	CG	MET	1095	11.242	13.507	5.999		28.03	6
ATOM	2086	SD	MET	1095	12.707	14.551	6.044	1.00	28.03	16
ATOM	2087	CE	MET	1095	13.094	14.706	4.302	1.00	28.03	6
ATOM	2088	C	MET	1095	7.757	13.989	5.274	1.00	51.73	6
ATOM	2089	0	MET	1095	7.425	13.870	6.450	1.00	51.73	8
ATOM	2090	N	LEU	1096	7.123	14.763	4.413		48.50	7
ATOM	2091	CA	LEU	1096	5.981	15.557	4.825		48.50	6
ATOM	2092	CB	LEU	1096	5.889	16.790	3.951		41.93	6
MOTA	2093	CG	LEU	1096	6.365	18.048	4.638		41.93	6
ATOM	2094		LEU	1096	6.177	19.139	3.616		41.93	6
ATOM	2095	CD2	LEU	1096	5.593	18.342	5.911		41.93	6
ATOM	2096	C	LEU	1096	4.663	14.859	4.783		48.50	6
ATOM	2097	0	LEU	1096	3.747	15.199	5.536	1.00	48.50	8

ATOM	2098	N	GLU	1097	4.537	13.900	3.890	1.00 62.96	7
ATOM	2099	CA	GLU	1097	3.261	13.252	3.809	1.00 63.28	6
ATOM	2100	CB	GLU	1097	3.046	12.672	2.424	1.00 90.58	6
ATOM	2101	CG	GLU	1097	2.625	13.708	1.449	1.00 90.58	6
ATOM	2102	CD	GLU	1097	2.523	13.139	0.080	1.00 90.58	6
ATOM	2103	OE1		1097	3.480	12.481	-0.333	1.00 90.58	8
ATOM	2104	OE2		1097	1.492	13.317	-0.587	1.00 90.58	8
ATOM	2105	C	GLU	1097	3.099	12.216	4.892	1.00 90.58	6
ATOM	2106	ō	GLU	1097	2.839	11.051	4.616		
ATOM	2107	N	GLU	1098	3.279	12.659		1.00 67.39	8
ATOM	2108	CA	GLU	1098	3.132		6.137	1.00 99.89	7
ATOM	2109	CB	GLU	1098	4.342	11.782	7.288	1.00 99.89	6
ATOM	2110	CG	GLU	1098	4.908	10.880	7.434	1.00 62.46	6
ATOM	2111	CD	GLU	1098		10.367	6.157	1.00 62.46	6
ATOM	2112		GLU	1098	 6.147	9.556	6.415	1.00 62.46	6
ATOM	2112		GLU		6.614	9.586	7.576	1.00 62.46	8
ATOM	2113	C	GLU	1098	6.653	8.914	5.474	1.00 62.46	8
ATOM	2114			1098	2.928	12.540	8.608	1.00 99.89	6
		0	GLU	1098	1.962	12.277	9.312	1.00 99.89	8
ATOM	2116	N	ARG	1099	3.815	13.483	8.937	1.00100.00	7
ATOM	2117	CA	ARG	1099	3.735	14.251	10.201	1.00100.00	6
ATOM	2118	CB	ARG	1099	2.339	14.863	10.443	1.00 95.05	6
ATOM	2119	CG	ARG	1099	2.140	15.416	11.871	1.00 83.68	6
ATOM	2120	CD	ARG	1099	3.239	16.413	12.239	1.00 83.68	6
ATOM	2121	NE	ARG	1099	3.123	16.915	13.609	1.00 83.68	7
MOTA	2122	CZ	ARG	1099	3.314	18.185	13.955	1.00 83.68	6
ATOM	2123		ARG	1099	3.636	19.072	13.024	1.00 83.68	7
ATOM	2124		ARG	1099	3.179	18.572	15.222	1.00 83.68	7
ATOM	2125	C	ARG	1099	4.083	13.322	11.354	1.00100.00	6
ATOM	2126	0	ARG	1099	3.393	13.259	12.370	1.00100.00	8
ATOM	2127	N	LYS	1100	5.153	12.570	11.174	1.00 88.41	7
ATOM	2128	CA	LYS	1100	5.572	11.681	12.224	1.00 88.41	6
ATOM	2129	CB	LYS	1100	6.250	10.454	11.641	1.00 87.41	6
ATOM	2130	CG	LYS	1100	5.322	9.628	10.762	1.00 87.41	6
ATOM	2131	CD	LYS	1100	3.984	9.336	11.456	1.00 87.41	6
ATOM	2132	CE	LYS	1100	4.165	8.742	12.861	1.00 59.92	6
ATOM	2133	NZ	LYS	1100	4.852	7.411	12.877	1.00 59.92	7
ATOM	2134	C	LYS	1100	6.519	12.453	13.123	1.00 88.41	6
MOTA	2135	0	LYS	1100	7.597	11.969	13.470	1.00 88.41	8
ATOM	2136	N	THR	1101	6.112	13.672	13.472	1.00100.00	7
ATOM	2137	CA	THR	1101	6.892	14.519	14.356	1.00100.00	6
ATOM	2138	CB	THR	1101	6.795	13.998	15.811	1.00100.00	6
ATOM	2139		THR	1101	5.426	14.034	16.239	1.00 90.24	8
MOTA	2140		THR	1101	7.652	14.836	16.750	1.00 90.24	6
ATOM	2141	С	THR	1101	8.362	14.565	13.927	1.00100.00	6
ATOM	2142	0	THR	1101	9.219	13.923	14.541	1.00100.00	8
ATOM	2143	N	TYR	1102	8.655	15.300	12.862	1.00 39.18	7
ATOM	2144	CA	TYR	1102	10.042	15.411	12.416	1.00 39.18	6
ATOM	2145	CB	TYR	1102	10.106	15.624	10.912	1.00 91.13	6
ATOM	2146	CG	TYR	1102	9.798	14.391	10.132	1.00 60.67	6
ATOM	2147	CD1	TYR	1102	8.500	14.112	9.717	1.00 60.67	6
ATOM	2148		TYR	1102	8.222	12.956	9.006	1.00 60.67	6
ATOM	2149	CD2	TYR	1102	10.809	13.487	9.821	1.00 60.67	6
ATOM	2150	CE2	TYR	1102	10.544	12.338	9.120	1.00 60.67	6
ATOM	2151	CZ	TYR	1102	9.256	12.078	8.711	1.00 60.67	6
ATOM	2152	OH	TYR	1102	9.019	10.950	7.978	1.00 60.67	8
ATOM	2153	C	TYR	1102	10.781	16.549	13.102	1.00 39.18	6
ATOM	2154	0	TYR	1102	12.003	16.594	13.090	1.00 39.18	8

VAL 1103 2156 CA VAL 1103

VAL 1103

2157 CB VAL 1103

2158 CG1 VAL 1103

2159 CG2 VAL 1103

2160 C VAL 1103

2162 N ASN 1104

MOTA

ATOM

MOTA MOTA

ATOM

MOTA

ATOM

2204 O GLU 1109

2205 N LYS 1110

2206 CA LYS 1110

2207 CB LYS 1110 2208 CG LYS 1110

2209 CD LYS 1110

2210 CE LYS 1110

2211 NZ LYS 1110

2155 N

2161 0

	ALON	2102	7.4	1470TA	T T O 4	10.343	10.3/0	10.707	1.00	01.07
	ATOM	2163	CA	ASN	1104	9.624	18.773	18.003	1.00	61.67
	ATOM	2164	CB	ASN	1104	10.315	18.015	19.112	1.00	93.99
	MOTA	2165	CG	ASN	1104	9.344	17.404	20.054	1.00	53.82
	ATOM	2166	OD1	ASN	1104	8.643	18.111	20.791	1.00	53.82
	ATOM	2167	ND2	ASN	1104	9.261	16.076	20.028	1.00	53.82
	ATOM	2168	C	ASN	1104	 9.470	20.240	18.395	1.00	61.67
	ATOM	2169	0	ASN	1104	10.453	20.966	18.484	1.00	61.67
	ATOM	2170	N	THR	1105	8.233	20.675	18.625	1.00	43.79
	ATOM	2171	ÇA	THR	1105	7.960	22.059	19.024	1.00	43.79
	ATOM	2172	CB	THR	1105	7.081	22.763	18.002	1.00	95.52
	ATOM	2173	OG1	THR	1105	5.888	22.001	17.786	1.00	51.15
	ATOM	2174	CG2	THR	1105	7.835	22.923	16.700	1.00	51.15
[3]	ATOM	2175	C	THR	1105	7.231	22.045	20.350	1.00	43.79
Ú.	ATOM	2176	0	THR	1105	6.598	23.024	20.754	1.00	43.79
CO.	ATOM	2177	N	THR	1106	7.338	20.905	21.016	1.00	47.73
erië.	ATOM	2178	CA	THR	1106	6.683	20.671	22.281	1.00	47.73
LI)	ATOM	2179	CB	THR	1106	5.850	19.415	22.236	1.00	24.03
1,0,1	MOTA	2180	OG1	THR	1106	4.835	19.542	21.237	1.00	24.03
100 mg	ATOM	2181	CG2	THR	1106	5.222	19.167	23.580	1.00	24.03
12	ATOM	2182	C	THR	1106	7.676	20.434	23.372	1.00	47.73
	ATOM	2183	0	THR	1106	8.742	19.880	23.129	1.00	47.73
	ATOM	2184	N	LEU	1107	7.311	20.833	24.583	1.00	64.31
	ATOM	2185	CA	LEU	1107	8.174	20.612	25.723	1.00	64.31
141	ATOM	2186	CB	LEU	1107	8.207	21.803	26.637	1.00	96.32
M.	ATOM	2187	CG	LEU	1107	8.957	22.900	25.957	1.00	40.62
NU	ATOM	2188		LEU	1107	7.919	23.838	25.432	1.00	40.62
0	ATOM	2189	CD2	LEU	1107	9.864	23.587	26.914	1.00	40.62
44	ATOM	2190	C	LEU	1107	7.795	19.433	26.564	1.00	64.31
	ATOM	2191	0	LEU	1107	6.801	19.458	27.281	1.00	64.31
	ATOM	2192	N	TYR	1108	8.708	18.463	26.384	1.00	94.02
	MOTA	2193	CA	TYR	1108	8.405	17.305	27.238	1.00	94.02
	ATOM	2194	CB	TYR	1108	8.596	16.009	26.448	1.00	99.65
	ATOM	2195	CG	TYR	1108	7.705	15.929	25.207	1.00	78.77
	ATOM	2196	CD1	TYR	1108	7.913	14.643	24.404	1.00	78.77
	ATOM	2197	CD2	TYR	1108	6.212	15.974	25.538	1.00	78.77
	ATOM	2198	C	TYR	1108	9.340	17.291	28.449	1.00	94.02
	ATOM	2199	0	TYR	1108	8.922	16.976	29.574	1.00	94.02
	ATOM	2200	N	GLU	1109	10.796	17.582	27.521	1.00	92.55
	MOTA	2201	CA	GLU	1109	11.496	17.815	28.793	1.00	92.55
	MOTA	2202	CB	GLU	1109	11.234	16.655	29.755		95.82
	ATOM	2203	C	GLU	1109	13.002	17.927	28.549	1.00	92.55

054 1.00 53.82 6 791 1.00 53.82 028 1.00 53.82 7 395 1.00 61.67 484 1.00 61.67 .625 1.00 43.79 .024 1.00 43.79 .002 1.00 95.52 .786 1.00 51.15 .700 1.00 51.15 .350 1.00 43.79 .754 1.00 43.79 .016 1.00 47.73 7 .281 1.00 47.73 .236 1.00 24.03 .237 1.00 24.03 В .580 1.00 24.03 .372 1.00 47.73 .129 1.00 47.73 .583 1.00 64.31 723 1.00 64.31 637 1.00 96.32 957 1.00 40.62 6 .432 1.00 40.62 .914 1.00 40.62 .564 1.00 64.31 .281 1.00 64.31 .384 1.00 94.02 238 1.00 94.02 6 .448 1.00 99.65 6 207 1.00 78.77 6 .404 1.00 78.77 6 .538 1.00 78.77 6 .449 1.00 94.02 .574 1.00 94.02 9 521 1.00 92.55 7 793 1.00 92.55 755 1.00 95.82 .549 1.00 92.55 13.672 16.935 28.226 1.00 92.55 13.581 19.231 28.669 1.00 54.62 7 14.995 19.556 28.430 1.00 54.62 15.850 18.294 28.564 1.00100.00 16.129 17.914 30.020 1.00 99.80 6 17.313 16.956 30.171 1.00 99.80 6 17.333 16.240 31.523 1.00 99.80 6 18.525 15.400 31.710 1.00 99.80 FIG. 3MM

10.028 17.469 13.690 1.00 80.69 10.614 18.614 14.370 1.00 80.69 10.585 19.857 13.466 1.00 82.85 11.221 21.042 14.165 1.00 25.69

11.310 19.563 12.172 1.00 25.69

9.791 18.892 15.611 1.00 80.69

8.677 19.395 15.529 1.00 80.69

10.345 18.570 16.767 1.00 61.67

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Docket/App No.: 2079.1037-001

Title: Method of Identifying Inhibitors of TIE-2 Inventors: Nancy J. Bump *et al.*

ATOM 2212 C LYS 1110 15.168 20.134 27.023 1.00 54.62 ATOM 2214 N PHE 1111 14.506 21.258 26.825 1.00 53.78 ATOM 2215 CA PHE 1111 14.507 21.258 26.825 1.00 53.78 ATOM 2216 CB PHE 1111 14.527 21.994 25.551 1.00 53.78 ATOM 2216 CB PHE 1111 13.144 22.558 25.259 1.00 97.53 ATOM 2217 CG PHE 1111 13.144 22.558 25.259 1.00 97.53 ATOM 2218 CD1 PHE 1111 12.847 22.718 23.764 1.00 42.19 ATOM 2218 CD1 PHE 1111 12.847 22.718 23.764 1.00 42.19 ATOM 2219 CD2 PHE 1111 12.868 21.651 23.023 1.00 42.19 ATOM 2219 CD2 PHE 1111 12.068 21.651 23.023 1.00 42.19 ATOM 2220 CE1 PHE 1111 12.078 24.100 21.773 1.00 42.19 ATOM 2221 CE2 PHE 1111 12.798 24.100 21.773 1.00 42.19 ATOM 2221 CE2 PHE 1111 12.798 24.100 21.773 1.00 42.19 ATOM 2222 C PHE 1111 12.528 23.149 25.661 1.00 53.78 ATOM 2223 C PHE 1111 15.647 23.812 26.681 1.00 53.78 ATOM 2224 C PHE 1111 15.647 23.812 26.681 1.00 53.78 ATOM 2224 C PHE 1111 15.647 23.812 26.681 1.00 53.78 ATOM 2229 CG THR 1112 17.246 24.596 24.296 1.00 41.67 ATOM 2229 CG THR 1112 17.246 24.596 24.296 1.00 81.88 ATOM 2229 CG THR 1112 17.246 24.596 24.296 1.00 81.18 ATOM 2228 CG THR 1112 18.657 22.952 23.224 1.00 84.38 ATOM 2230 C THR 1112 18.657 22.952 23.224 1.00 84.38 ATOM 2231 C THR 1112 18.657 22.952 23.224 1.00 84.38 ATOM 2233 C THR 1112 18.657 22.952 23.224 1.00 84.38 ATOM 2233 C THR 1112 18.657 22.952 23.255 1.00 88.60 10 ATOM 2233 C THR 1113 17.729 26.628 23.155 1.00 88.60 10 ATOM 2233 C THR 1113 17.729 26.628 23.155 1.00 88.60 10 ATOM 2234 C THR 1113 17.729 26.628 23.155 1.00 88.60 10 ATOM 2234 C THR 1113 17.729 27.664 22.034 1.00 81.65 ATOM 2235 CG TYR 1113 17.729 26.628 23.155 1.00 88.60 10 ATOM 2234 C THR 1113 17.729 27.664 22.034 1.00 81.65 ATOM 2235 CG TYR 1113 17.729 27.664 22.034 1.00 88.60 10 ATOM 2234 C THR 1113 17.729 27.664 22.034 1.00 88.60 10 ATOM 2234 C THR 1113 17.729 27.664 22.034 1.00 88.60 10 ATOM 2234 C THR 1113 17.729 27.664 22.034 1.00 88.60 10 ATOM 2234 C THR 1113 17.729 27.664 22.034 1.00 88.60 10 ATOM 2235 CG TYR 1113 17.729 27.664 22.034 1.00 88.60 10 ATOM 2235 CG TYR 1113 17.72 MOTA 2212 C LYS 1110 15.168 20.134 27.023 1.00 54.62 7 TER TER HETATM 2259 C29 TEM 1 14.137 43.777 -1.896 1.00 87.75 HETATM 2260 C130 TEM 1 15.517 44.384 -2.200 1.00 92.68 HETATM 2261 C31 TEM 1 13.532 43.996 -0.603 1.00 84.61 HETATM 2262 C32 TEM 1 10.062 43.539 1.417 1.00 72.29 HETATM 2263 C28 TEM 1 13.152 42.505 -7.029 1.00 92.68 HETATM 2264 C8 TEM 1 11.669 44.356 4.626 1.00 64.60 HETATM 2265 C9 TEM 1 12.234 43.146 5.418 1.00 62.65 HETATM 2266 C10 TEM 1 12.979 43.794 6.609 1.00 61.60 HETATM 2267 C11 TEM 1 13.328 45.233 6.175 1.00 61.11

2268	C12	TEM	1	12.788	45.420	4.740	1.00	62.68	6
2269	C13	TEM	1	12.175	43.912	2.185	1.00	71.00	6
2270	N7	TEM	1	11.303	44.043	3.228	1.00	67.78	7
2271	N1	TEM	1	8.672	43.004	-0.559	1.00	73.02	7
2272	C2	TEM	1	8.784	43.270	0.784	1.00	71.64	6
2273	N3	TEM	1	7.669	43.306	1.546	1.00	71.42	7
2274	C4	TEM	1	7.718	43.568	2.851	1.00	69.68	6
2275	N5	TEM	1	8.853	43.811	3.473	1.00	68.84	7
2276	C6	TEM	1	10.030	43.817	2.820	1.00	69.92	6
2277	C14	TEM	1	11.530	43.630	1.036	1.00	75.68	6
2278	022	TEM	1	13.956	40.236	-4.115	1.00	92.68	8
2279	C23	TEM	1	13.420	41.285	-6.355	1.00	92.68	6
2280	C24	TEM	1	12.844	40.071	-6.856	1.00	92.68	6
2281	C25	TEM	1	12.014	40.102	-8.027	1.00	92.68	6
2282	C26	TEM	1	11.757	41.334	-8.689	1.00	92.68	6
2283	C27	TEM	1	12.330	42.534	-8.187	1.00	92.68	6
2284	021	TEM	1	15.786	41.592	-5.276	1.00	92.68	8
2285	C15	TEM	1	12.216	43.429	-0.313	1.00	80.63	6
2286	C16	TEM	1	11.576	42.675	-1.308	1.00	83.45	6
2287	C17	TEM	1	12.141	42.492	-2.551	1.00	87.27	6
2288	C18	TEM	1	13.399	43.018	-2.887	1.00	88.78	б
2289	N19	TEM	1	13.818	42.732	-4.220	1.00	90.27	7
2290	S20	TEM	1	14.444	41.335	-4.875	1.00	92.68	16
2291	S	S04	2	25.361	40.893	-8.736	1.00	15.55	16
2292	01	SO4	2	26.331	39.742	-8.499	1.00	20.26	8
2293	02	S04	2	25.230	41.131	-10.222	1.00	12.30	8
2294	03	SO4	2	23.982	40.607	-8.171	1.00	16.39	8
2295	04	SO4	2	25.930	42.110	-8.051	1.00	17.72	8
	2270 2271 2272 2273 2274 2276 2277 2278 2280 2281 2282 2283 2284 2288 2288 2288 2288 2289 2281 2292 2291 2292	2669 C13 C270 N7 C2771 N1 C2772 C2 C273 N3 C274 C4 C275 N5 C276 C275 C276 C2779 C14 C278 C2779 C14 C278 C278	200 13 TEM	200 201 TEM	2266 C13 TEM	12.175	12-17 24-91 2-185 2-185 2-270 N7 TEM 1		12.175

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ATOM

67 CD1 ILE A 824

ATOM 1 N VAL A 818 77,669 47.027 2.354 1.00 20.00 ATOM 2 CA VAL A 818 76.422 47.479 1.690 1.00 20.00 ATOM 3 C VAL A 818 75.257 46.471 1,737 1,00 20,00 75.361 45.363 ATOM 4 O VAL A 818 2.335 1.00 20.00 5 CB VAL A 818 76.716 47.863 ATOM 0.250 1.00 20.00 ATOM 9 N LEU A 819 74.145 46.870 1.095 1.00 20.00 ATOM 10 CA LEU A 819 72.922 46.055 1.058 1.00 20.00 ATOM 11 C LEU A 819 72.341 45.959 -0.347 1.00 20.00 71.187 46.223 -0.571 1.00 20.00 ATOM 12 O LEU A 819 71.897 46.637 ATOM 13 CB LEU A 819 2.052 1.00 20.00 ATOM 14 CG LEU A 819 70.399 46.340 1.987 1.00 20.00 MOTA 15 CD1 LEU A 819 70.026 45.327 3.039 1.00 20.00 69,612 47,643 ATOM 16 CD2 LEU A 819 2.186 1.00 20.00 ATOM 18 N ASP A 820 73.165 45.565 -1.294 1.00 20.00 72.758 45.427 19 CA ASP A 820 -2.685 1.00 20.00 ATOM 72.758 45.427 -2.685 1.00 20.00 71.419 45.961 -3.188 1.00 20.00 70.510 45.182 -3.445 1.00 20.00 72.687 43.971 -3.103 1.00 20.00 72.637 43.799 -4.570 1.00 20.00 72.617 42.622 -5.045 1.00 20.00 ATOM 20 C ASP A 820 ATOM 21 0 ASP A 820 22 CB ASP A 820 ATOM 23 CG ASP A 820 ATOM ATOM 24 OD1 ASP A 820 ATOM 25 OD2 ASP A 820 72.468 44.861 -5.242 1.00 20.00 ATOM 27 N TRP A 821 71.336 47.280 -3.390 1.00 20.00 ATOM 28 CA TRP A 821 70.128 47.958 -3.916 1.00 20.00 ATOM 29 C TRP A 821 69.296 47.063 -4.814 1.00 20.00 ATOM 30 0 TRP A 821 68.077 47.237 -4.938 1.00 20.00 ATOM 31 CB TRP A 821 70.479 49.190 -4.782 1.00 20.00 ATOM 32 CG TRP A 821 69.336 50.211 -4.771 1.00 20.00 ATOM 33 CD1 TRP A 821 68.872 50.892 -3.675 1.00 20.00 ATOM 34 CD2 TRP A 821 68.465 50.552 -5.841 1.00 20.00 ATOM 35 NE1 TRP A 821 67.753 51.628 -4.001 1.00 20.00 ATOM 36 CE2 TRP A 821 67.482 51.435 -5.325 1.00 20.00 ATOM 37 CE3 TRP A 821 68.408 50.201 -7.177 1.00 20.00 38 CZ2 TRP A 821 ATOM 66.462 51.963 -6.104 1.00 20.00 ATOM 39 CZ3 TRP A 821 67.382 50.730 -7.962 1.00 20.00 ATOM 40 CH2 TRP A 821 66,430 51,597 -7,420 1,00 20,00 MOTA 43 N ASN A 822 69.999 46.156 -5.498 1.00 20.00 69.370 45.213 -6.404 1.00 20.00 67.947 44.823 -5.911 1.00 20.00 67.000 44.734 -6.707 1.00 20.00 70.291 43.986 -6.531 1.00 20.00 ATOM 44 CA ASN A 822 ATOM 45 C ASN A 822 ATOM 46 O ASN A 822 70.291 43.986 -6.531 1.00 20.00 69.810 42.766 -7.181 1.00 20.00 69.406 41.706 -8.393 1.00 20.00 69.406 41.706 -6.377 1.00 20.00 69.406 41.706 -6.377 1.00 20.00 66.472 44.212 -4.129 1.00 20.00 66.472 44.212 -4.129 1.00 20.00 66.179 44.295 -1.758 1.00 20.00 66.179 44.295 -1.758 1.00 20.00 66.179 44.295 -1.758 1.00 20.00 66.179 44.295 -2.988 1.00 20.00 66.179 44.295 -1.758 1.00 20.00 66.179 44.295 -1.758 1.00 20.00 66.179 45.506 45.894 -2.988 1.00 20.00 65.166 45.894 -2.988 1.00 20.00 65.166 45.894 -1.859 1.00 20.00 65.666 48.804 6.524 -1.859 1.00 20.00 65.666 48.876 -2.883 1.00 20.00 65.666 48.876 -2.883 1.00 20.00 65.666 48.876 -2.883 1.00 20.00 65.865 48.113 -0.382 1.00 20.00 67.135 48.549 -2.681 1.00 20.00 ATOM 47 CB ASN A 822 ATOM 48 CG ASN A 822 ATOM 49 OD1 ASN A 822 ATOM 50 ND2 ASN A 822 ATOM 54 N ASP A 823 ATOM 55 CA ASP A 823 ATOM 56 C ASP A 823 ATOM 57 O ASP A 823 58 CB ASP A 823 ATOM 60 N ILE A 824 ATOM 61 CA ILE A 824 62 C ILE A 824 63 O ILE A 824 MOTA ATOM ATOM 64 CB ILE A 824 ATOM ATOM 65 CG1 ILE A 824 66 CG2 ILE A 824 MOTA

Docket/App No.: 2079.1037-001

Title: Method of Identifying Inhibitors of TIE-2 Inventors: Nancy J. Bump *et al.*

ATOM	69	N	LYS	Α	825	62.077	45.969	-1.626	1.00 20.00
ATOM	70	CA	LYS			60.645	45.921	-2.029	1.00 20.00
ATOM	71	C	LYS			59.922	47.060	-1.266	1.00 20.00
ATOM	72	ō	LYS			59.578	46.946	-0.097	1.00 20.00
ATOM	73	CB	LYS			60.043	44.561	-1.696	1.00 20.00
ATOM	75	N	PHE			59.696	48.147	-1.988	1.00 20.00
ATOM	76	CA	PHE		826	59.153	49.401	-1.462	1.00 20.00
ATOM	77	C	PHE		826	57.643	49.569	-1.593	1.00 20.00
ATOM	7.8	ō			826	57.160	50.073	-2.593	1.00 20.00
ATOM	79	CB			826	59.882	50.481	-2.224	1.00 20.00
ATOM	80	CG	PHE			60.298	50.013	-3.604	1.00 20.00
ATOM	81	CD1			826	59.336	49.841	-4.613	1.00 20.00
ATOM	82	CD2	PHE			61.611	49.711	-3.887	1.00 20.00
ATOM	83	CE1	PHE			59.675	49.711	-5.876	1.00 20.00
ATOM	84	CE2	PHE			61.960	49.249	-5.145	1.00 20.00
ATOM	85	CZ	PHE						
						60.984	49.086	-6.144	1.00 20.00
ATOM	87	N	GLN			56.919	49.173	-0.550	1.00 20.00
ATOM	88	CA	GLN			55.459	49.206	-0.491	1.00 20.00
ATOM	89	C	GLN			54.788	50.547	-0.268	1.00 20.00
ATOM	90	0	GLN			54.134	51.071	-1.177	1.00 20.00
ATOM	91	CB	GLN		827	54.978	48.268	0.591	1.00 20.00
ATOM	92	CG	GLN		827	56.111	47.581	1.340	1.00 20.00
ATOM	93	CD	GLN			56.511	46.315	0.637	1.00 20.00
ATOM	94	OE1	GLN			56.636	45.253	1.256	1.00 20.00
ATOM	95	NE2	GLN			56.688	46.410	-0.675	1.00 20.00
ATOM	99	N	ASP			54.918	51.103	0.928	1.00 20.00
ATOM	100	CA	ASP			54.261	52.360	1.165	1.00 20.00
ATOM	101	C	ASP			54.815	53.309	2.231	1.00 20.00
ATOM	102	0			828	55.694	52.973	3.033	1.00 20.00
ATOM	103	CB	ASP			52.856	52.049	1.499	1.00 20.00
ATOM	104	CG	ASP			52.783	50.948	2.460	1.00 20.00
ATOM	105		ASP			52.099	49.943	2.182	1.00 20.00
ATOM	106	OD2	ASP			53.439	51.088	3.504	1.00 20.00
ATOM	108	N	VAL		829	54.278	54.522	2.216	1.00 20.00
ATOM	109	CA	VAL			54.681	55.525	3.158	1.00 20.00
ATOM	110	C	VAL			54.405	54.794	4.471	1.00 20.00
ATOM	111	0	VAL			53.373	54.176	4.562	1.00 20.00
ATOM	112	CB	VAL			53.772	56.742	2.971	1.00 20.00
ATOM	114	N	ILE			55.298	54.759	5.453	1.00 20.00
ATOM	115	CA	ILE			54.911	54.062	6.686	1.00 20.00
ATOM	116	C	ILE			54.690	55.170	7.627	1.00 20.00
ATOM	117	0	ILE			55.296	55.229	8.696	1.00 20.00
ATOM	118	CB	ILE			56.004	53.170	7.366	1.00 20.00
ATOM	119	CG1	ILE			56.458	52.054	6.437	1.00 20.00
ATOM	120	CG2	ILE			55.435	52.493	8.636	1.00 20.00
MOTA	121	CD1	ILE			57.626	51.361	6.996	1.00 20.00
ATOM	123	N	GLY			53.802	56.059	7.244	1.00 20.00
ATOM	124	CA	GLY			53.588	57.205	8.087	1.00 20.00
ATOM	125	C	GLY			54.694	58.162	7.693	1.00 20.00
ATOM	126	0	GLY			55.359	57.972	6.691	1.00 20.00
ATOM	128	N	GLU			54.888	59.180	8.505	1.00 20.00
ATOM	129	CA	GLU			55.889	60.205	8.260	1.00 20.00
ATOM	130	C	GLU			57.146	59.876	7.452	1.00 20.00
ATOM	131	0_	GLU			57.220	58.893	6.667	1.00 20.00
ATOM	132	CB	GLU			56.346	60.832	9.592	1.00 20.00
ATOM	133	CG	GLU			56.473	62.337	9.489	1.00 20.00
ATOM	134	CD	GLU	A	832	55.501	62.908	8.468	1.00 20.00

ATOM	135	OE1	GLU	А	832	54.643	63.721	8.897	1.00 20.00
ATOM	136	OE2	GLU			55.599	62.524	7.266	1.00 20.00
MOTA	138	N	GLY			58.134	60.754	7.680	1.00 20.00
ATOM	139	CA	GLY			59.440	60.670	7.054	1.00 20.00
ATOM	140	c	GLY			60.222	61.871	7.561	1.00 20.00
ATOM	141	ō			833	60.606	61.957	8.770	1.00 20.00
ATOM	143	N	ASN			60.380	62.816	6.621	1.00 20.00
ATOM	144	CA	ASN			61.123	64.085	6.772	1.00 20.00
ATOM	145	C	ASN			62.555	63.797	7.139	1.00 20.00
ATOM	146	ō	ASN			62.796	63.133	8.141	1.00 20.00
ATOM	147	CB	ASN			60.584	65.052	7.859	1.00 20.00
ATOM	148	CG	ASN			61.664	66.125	8.258	1.00 20.00
ATOM	149	OD1	ASN	Α	834	61.998	66.999	7.444	1.00 20.00
ATOM	150		ASN			62.224	66.022	9.491	1.00 20.00
ATOM	154	N	PHE			63.474	64.373	6.355	1.00 20.00
ATOM	155	CA	PHE	Ā	835	64.922	64.216	6.526	1.00 20.00
ATOM	156	С	PHE		835	64.972	63.040	7.488	1.00 20.00
ATOM	157	0	PHE			65.560	63.063	8.616	1.00 20.00
ATOM	158	CB	PHE	Α	835	65.545	65.547	7.028	1.00 20.00
ATOM	159	CG			835	65.828	66.560	5.895	1.00 20.00
ATOM	160	CD1			835	65.442	67.913	6.013	1.00 20.00
ATOM	161	CD2	PHE	Α	835	66.534	66.176	4.742	1.00 20.00
ATOM	162	CE1	PHE			65.761	68.870	5.004	1.00 20.00
ATOM	163	CE2	PHE			66.859	67.138	3.725	1.00 20.00
ATOM	164	CZ	PHE			66.469	68.482	3.867	1.00 20.00
ATOM	166	N	GLY			64.251	62.029	6.984	1.00 20.00
ATOM	167	CA	GLY	А	836	64.025	60.759	7.647	1.00 20.00
ATOM	168	С	GLY	Α	836	62.817	60.226	6.884	1.00 20.00
ATOM	169	0	GLY	Α	836	61.874	59.661	7.452	1.00 20.00
MOTA	171	N	GLN	Α	837	62.827	60.432	5.571	1.00 20.00
ATOM	172	CA	GLN	Α	837	61.720	59.959	4.749	1.00 20.00
ATOM	173	C	GLN	A	837	61.471	58.496	5.132	1.00 20.00
ATOM	174	0	GLN	Α	837	62.278	57.647	4.742	1.00 20.00
MOTA	175	CB	GLN	Α	837	62.112	60.066	3.253	1.00 20.00
ATOM	176	CG	GLN	A	837	63.459	60.807	2.984	1.00 20.00
ATOM	177	CD	GLN	Α	837	63.541	61.552	1.605	1.00 20.00
ATOM	178	OEl	GLN	А	837	64.298	62.539	1.447	1.00 20.00
MOTA	179	NE2	GLN	Α	837	62.786	61.053	0.607	1.00 20.00
ATOM	183	N	VAL	Α	838	60.400	58.162	5.872	1.00 20.00
ATOM	184	CA	VAL	Α	838	60.233	56.718	6.211	1.00 20.00
ATOM	185	С	VAL	Α	838	59.296	55.833	5.400	1.00 20.00
ATOM	186	0	VAL	А	838	58.143	55.705	5.734	1.00 20.00
ATOM	187	CB	VAL	Α	838	59.824	56.442	7.659	1.00 20.00
ATOM	188	CG1	VAL	A	838	60.786	55.456	8.230	1.00 20.00
ATOM	189	CG2	VAL	Α	838	59.760	57.703	8.475	1.00 20.00
MOTA	191	N	LEU	Α	839	59.820	55.181	4.373	1.00 20.00
ATOM	192	CA	LEU	Α	839	59.031	54.306	3.542	1.00 20.00
ATOM	193	C	LEU	А	839	58.983	52.882	4.069	1.00 20.00
MOTA	194	0	LEU	Α	839	59.676	52.547	5.015	1.00 20.00
ATOM	195	CB	LEU	Α	839	59.566	54.385	2.111	1.00 20.00
ATOM	196	CG	LEU			58.912	55.608	1.396	1.00 20.00
ATOM	197		LEU			58.295	56.545	2.426	1.00 20.00
ATOM	198	CD2	LEU	Α	839	59.886	56.367	0.533	1.00 20.00
MOTA	200	N	LYS		840	58.119	52.049	3.503	1.00 20.00
MOTA	201	CA		A	840	58.031	50.646	3.945	1.00 20.00
ATOM	202	C	LYS			58.687	49.724	2.927	1.00 20.00
ATOM	203	0	LYS	Α	840	58.645	49.971	1.725	1.00 20.00

ATOM	204	CB	LYS	Α	840	56.577	50.198	4.145	1.00	20.00
ATOM	205	CG	LYS			56.445	49.166	5.251		20.00
ATOM	206	CD	LYS			55.843	47.830	4.789		20.00
ATOM	207	CE	LYS			55.173	47.110	5.960		20.00
ATOM	208	NZ	LYS			56.154				20.00
							46.444	6.801		
ATOM	213	N	ALA			59.302	48.650	3.383		20.00
ATOM	214	CA	ALA			59.929	47.798	2.393		20.00
ATOM	215	C	ALA			60.199	46.360	2.787		20.00
MOTA	216	0	ALA			60.460	46.044	3.971		20.00
ATOM	217	CB	ALA			61.224	48.462	1.884		20.00
MOTA	219	N	ARG	Α	842	60.111	45.506	1.759	1.00	20.00
ATOM	220	CA	ARG	Α	842	60.347	44.075	1.824	1.00	20.00
ATOM	221	C	ARG	Α	842	61.797	43.918	1.340	1.00	20.00
ATOM	222	0	ARG			62.105	43.967	0.158		20.00
ATOM	223	CB	ARG			59.365	43.360	0.902		20.00
ATOM	225	N	ILE			62.688	43.746	2.293		20.00
ATOM	226	CA	ILE			64.113	43.638	2.034		20.00
ATOM	227	C	ILE			64.747	42.223			20.00
								2.205		
ATOM	228	0	ILE			64.527	41.503	3.201		20.00
ATOM	229	CB	ILE			64.846	44.662	2.928		20.00
ATOM	230		ILE			65.867	45.411	2.103		20.00
ATOM	231	CG2				65.469	43.996	4.130		20.00
MOTA	232	CD1				66.176	44.779	0.772		20.00
MOTA	234	N	LYS	Α	844	65.549	41.837	1.226	1.00	20.00
ATOM	235	CA	LYS	Α	844	66.190	40.551	1.273	1.00	20.00
ATOM	236	C	LYS	Α	844	67.652	40.641	1.709	1.00	20.00
ATOM	237	0	LYS	Α	844	68.540	40.820	0.869	1.00	20.00
ATOM	238	CB	LYS	Α	844	66.093	39.875	-0.111	1.00	20.00
ATOM	240	N	LYS	Α	845	67.897	40.510	3.014		20.00
ATOM	241	CA	LYS			69.261	40.516	3.545		20.00
ATOM	242	C	LYS			69.917	39.112	3.335		20.00
ATOM	243	ō	LYS			69.306	38.060	3.678		20.00
ATOM	244	CB	LYS			69.255	40.857	5.035		20.00
ATOM	246	N								
ATOM	247	CA	ASP			71.148	39.140	2.765		20.00
			ASP			72.022	37.977	2.481		20.00
ATOM	248	C	ASP			71.224	36.671	2.559		20.00
ATOM	249	0	ASP			71.231	35.953	3.581		20.00
ATOM	250	CB	ASP			73.214	37.987	3.484		20.00
ATOM	251	CG	ASP			74.448	37.141	3.002	1.00	20.00
ATOM	252	OD1	ASP	Α	846	74.788	37.167	1.784	1.00	20.00
ATOM	253	OD2	ASP			75.078	36.450	3.869	1.00	20.00
ATOM	255	N	GLY	Α	847	70.497	36.405	1.476	1.00	20.00
ATOM	256	CA	GLY	Α	847	69.670	35.206	1.405	1.00	20.00
ATOM	257	C	GLY	Α	847	68.642	35.071	2.527	1.00	20.00
ATOM	258	0	GLY	Α	847	68.972	34.604	3.636		20.00
ATOM	260	N	LEU	Α	848	67.406	35.481	2.198		20.00
ATOM	261	CA	LEU	Z	848	66.192	35.495	3.049		20.00
ATOM	262	C	LEU			65.707	36.956	3.333		20.00
ATOM	263	0	LEU							
ATOM	264	CB				66.470	37.844	3.751		20.00
ATOM			LEU			66.402	34.666	4.318		20.00
	265	CG	LEU			66.559	35.338	5.653		20.00
ATOM	266		LEU			66.241	34.369	6.804		20.00
ATOM	267		LEU			68.011	35.849	5.755		20.00
MOTA	269	N	ARG			64.434	37.188	3.011		20.00
ATOM	270	CA	ARG			63.793	38.491	3.149		20.00
MOTA	271	C	ARG			63.495	38.916	4.576		20.00
MOTA	272	0	ARG	Α	849	63.795	38.195	5.542	1.00	20.00

Docket/App No.: 2079.1037-001

Inventors:

Nancy J. Bump et al.

ATOM 273 CB ARG A 849 62.465 38.508 2.388 1.00 20 00 ATOM 274 CG ARG A 849 62.570 38.136 0.936 1.00 20.00 ATOM 275 CD ARG A 849 61.348 38.648 0.182 1.00 20.00 ATOM 276 NE ARG A 849 61.060 37.918 -1.060 1.00 20.00 ATOM 277 CZ ARG A 849 60.337 36.795 -1.117 1.00 20.00 ATOM 278 NH1 ARG A 849 59.833 36.281 0.018 1.00 20.00 ATOM 279 NH2 ARG A 849 60.113 36.198 -2.308 1.00 20.00 ATOM 286 N MET A 850 62.903 40.112 4.678 1.00 20.00 ATOM 287 CA MET A 850 62.466 40.710 5.938 1.00 20.00 ATOM 288 C MET A 850 61.786 42.087 5.756 1.00 20.00 ATOM 289 O MET A 850 61.816 42.702 4.694 1.00 20.00 290 CB MET A 850 ATOM 63.628 40.814 65.005 41.061 6.953 1.00 20.00 ATOM 291 CG MET A 850 6.376 1.00 20.00 ATOM 292 SD MET A 850 66.205 41.855 7.507 1.00 20.00 ATOM 293 CE MET A 850 66.021 40.869 9.036 1.00 20.00 295 N ATOM ASP A 851 61.105 42.523 6.800 1.00 20.00 ATOM 296 CA ASP A 851 60.477 43.812 6.787 1.00 20.00 297 C ATOM ASP A 851 61.586 44.780 7.213 1.00 20.00 ATOM 298 0 ASP A 851 62.559 44.403 7.904 1.00 20.00 ATOM 299 CB ASP A 851 300 CG ASP A 851 59.381 43.909 7.855 1.00 20.00 58.154 43.076 7.546 1.00 20.00 57.886 42.769 6.352 1.00 20.00 ATOM ATOM 301 OD1 ASP A 851 ATOM 302 OD2 ASP A 851 57.452 42.744 8.545 1.00 20.00 ATOM 304 N ALA A 852 61.366 46.044 6.842 1.00 20.00 ATOM 305 CA ALA A 852 62.230 47.173 7.161 1.00 20.00 ATOM 306 C ALA A 852 61.483 48.457 6.814 1.00 20.00 61.483 48.487 6.814 1.00 20.00 60.631 48.480 5.902 1.00 20.00 63.507 47.092 6.332 1.00 20.00 61.774 49.522 7.546 1.00 20.00 61.205 50.818 7.189 1.00 20.00 ATOM 307 O ALA A 852 ATOM 308 CB ALA A 852 ATOM 310 N ALA A 853 ATOM 311 CA ALA A 853 MOTA 312 C ALA A 853 62.439 51.427 6.518 1.00 20.00 62.439 51.427 6.518 1.00 20.00 63.529 50.919 6.771 1.00 20.00 60.812 51.581 8.418 1.00 20.00 62.300 52.470 5.685 1.00 20.00 63.546 53.072 4.960 1.00 20.00 63.501 54.570 5.142 1.00 20.00 63.501 54.570 5.142 1.00 20.00 63.531 52.777 3.457 1.00 20.00 63.527 51.284 3.195 1.00 20.00 64.353 53.554 2.664 1.00 20.00 64.906 50.722 3.717 1.00 20.00 ATOM 313 O ALA A 853 ATOM 314 CB ALA A 853 ATOM 316 N ILE A 854 317 CA ILE A 854 318 C ILE A 854 ATOM MOTA 319 0 ATOM ILE A 854 ATOM 319 0 ILE A 854 ATOM 320 CB ILE A 854 ATOM 321 CG1 ILE A 854 ATOM 322 CG2 ILE A 854 ATOM 323 CD1 ILE A 854 ATOM 325 CD1 ILE A 854 64.906 50.722 3.717 1.00 20.00 64.699 55.189 5.023 1.00 20.00 ATOM 326 CA LYS A 855 64.901 56.684 5.158 1.00 20.00 ATOM 327 C LYS A 855 65.800 57.286 4.079 1.00 20.00 ATOM 328 O LYS A 855 65.740 56.867 2.946 1.00 20.00 ATOM 329 CB LYS A 855 65.417 57.088 6.580 1.00 20.00 6.792 1.00 20.00 8.262 1.00 20.00 8.917 1.00 20.00 ATOM 330 CG LYS A 855 66.949 57.267 ATOM 331 CD LYS A 855 67.333 57.776 ATOM 332 CE LYS A 855 68.597 57.022 ATOM 333 NZ LYS A 855 69.828 57.804 9.506 1.00 20.00 ATOM 338 N ARG A 856 66.573 58.311 4.439 1.00 20.00 ATOM 339 CA ARG A 856 67,569 59.035 3.573 1.00 20.00 ATOM 340 C ARG A 856 66.957 60.199 2.856 1.00 20.00 ATOM 341 O ARG A 856 66.375 60.027 1.793 1.00 20.00 342 CB ARG A 856 ATOM 342 CB ARG A 856 68.288 58.135 343 CG ARG A 856 69.278 58.948 68.288 58.135 2.533 1.00 20.00 ATOM 1.706 1.00 20.00 ATOM 344 CD ARG A 856

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ATOM	345	NE	ARG	Δ	856	68.8	R O	60.276	-0.435	1 00	20.00
ATOM	346	CZ	ARG		856	68.6		60.497	-1.732	1.00	
ATOM	347		ARG		856	68.4		59.484	-2.568	1.00	
ATOM	348	NH2	ARG		856	68.5		61.750	-2.204	1.00	
ATOM	355	N		A	857	67.1		61.381	3.446	1.00	
ATOM	356	CA			857	66.5		62.674	2.991	1.00	
ATOM	357	C			857	67.4		63.831	2.508	1.00	
ATOM	358	0			857	68.4		64.269	3.254		20.00
ATOM	359	CB	MET	А	857	65.6		63.220	4.125		20.00
ATOM	360	CG	MET	Α	857	64.2		63.699	3.730	1.00	
ATOM	361	SD	MET	Α	857	62.8		63.037	4.735	1.00	
ATOM	362	CE	MET	А	857	61.4		64.067	3.876		20.00
ATOM	363	OXT	MET	Α	857	67.1		64.316	1.383	1.00	
ATOM	365	N	ASP	Α	864	77.2		66.313	-0.527		20.00
ATOM	366	CA	ASP	Α	864	77.8		67.381	-1.394		20.00
ATOM	367	С	ASP	Α	864	78.5		68.418	-0.580	1.00	
ATOM	368	0	ASP	Α	864	79.6	19	68.925	-1.043	1.00	20.00
ATOM	369	CB	ASP	Α	864	76.7	68	68.105	-2.272	1.00	20.00
ATOM	373	N	ASP	Α	865	78.0	90	68.727	0.620	1.00	20.00
ATOM	374	CA	ASP	Α	865	78.7	09	69.760	1.436	1.00	20.00
ATOM	375	C	ASP	Α	865	78.1	28	69.958	2.819	1.00	20.00
ATOM	376	0	ASP	Α	865	78.8	44 '	70.418	3.695	1.00	20.00
MOTA	377	CB	ASP	Α	865	78.6	65	71.087	0.683	1.00	20.00
ATOM	379	N	HIS	Α	866	76.8	32	69.683	3.014	1.00	20.00
MOTA	380	CA	HIS	Α	866	76.2	23	69.807	4.364	1.00	20.00
ATOM	381	С	HIS	Α	866	76.4	25	68.436	4.955	1.00	20.00
MOTA	382	0	HIS	Α	866	76.5	37	68.227	6.178	1.00	20.00
ATOM	383	CB	HIS	Α	866	74.6	99 '	70.145	4.303	1.00	20.00
ATOM	384	CG	HIS	Α	866	73.8	36	69.068	3.706	1.00	20.00
ATOM	385	ND1	HIS	Α	866	73.5	11 (69.036	2.360	1.00	20.00
ATOM	386	CD2	HIS	Α	866	73.1	45	68.054	4.285	1.00	20.00
ATOM	387	CE1	HIS		866	72.6	53	68.054	2.140	1.00	20.00
ATOM	388	NE2	HIS			72.4		67.443	3.290	1.00	20.00
ATOM	392	N	ARG		867	76.4	81	67.523	3.992	1.00	20.00
ATOM	393	CA	ARG			76.6		66.101	4.167		20.00
ATOM	394	С			867	77.7		65.727	5.193	1.00	20.00
ATOM	395	0	ARG		867	78.9		65.919	4.933		20.00
ATOM	396	CB	ARG		867	77.0		65.491	2.804		20.00
ATOM	397	CG	ARG		867	78.0		66.314	2.001		20.00
ATOM	398	CD	ARG		867	79.5		66.134	2.438		20.00
ATOM	399	NE	ARG			80.4		67.048	1.682		20.00
ATOM	400	CZ	ARG			81.2		67.924	2.231		20.00
ATOM	401	NH1	ARG			81.3		68.025	3.566	1.00	20.00
ATOM	402	NH2	ARG			81.9		68.729	1.428	1.00	20.00
ATOM	409	N	ASP			77.3		65.205	6.345	1.00	20.00
MOTA	410	CA	ASP			78.1		64.729	7.417		20.00
ATOM	411	C			868	77.7		63.290	7.881		20.00
ATOM	412	0			868	77.7		62.981	9.089		20.00
ATOM	413	CB	ASP		868	78.1		65.733	8.593		20.00
ATOM	414	CG			868	77.4		65.248	9.815		20.00
ATOM	415	OD1			868	76.2		64.747	9.611		20.00
ATOM	416	QD2	ASP			77.9		65.385	10.971		20.00
ATOM	418	N	PHE		869	77.5		62.391	6.921		20.00
ATOM	419	CA	PHE		869	77.1		61.033	7.261		20.00
ATOM ATOM	420	C			869	78.0		59.895	6.841		20.00
ATOM	421 422	O CB	PHE		869	78.5		59.819	5.663		20.00
AION	422	CB	PRE	M	009	75.7	38 1	60.806	6.625	1.00	20.00

ATOM	423	CG	PHE	Α	869	75.685	61.221	5.199	1.00 20.00
ATOM	424	CD1	PHE			75.561	62.560	4.861	1.00 20.00
ATOM	425	CD2	PHE			75.848	60.286	4.190	1.00 20.00
MOTA	426	CE1	PHE	А	869	75.612	62.955	3.509	1.00 20.00
ATOM	427	CE2	PHE			75.896	60.680	2.838	1.00 20.00
ATOM	428	CZ	PHE			75.779	62.022	2.496	1.00 20.00
ATOM	430	N	ALA			78.350	59.018	7.812	1.00 20.00
MOTA	431	CA	ALA			79.231	57.831	7.715	1.00 20.00
ATOM	432	C	ALA			79.352	57.560	9.172	1.00 20.00
ATOM	433	ō	ALA			78.350	57.359	9.840	1.00 20.00
ATOM	434	CB	ALA			80.624	58.132	7.160	1.00 20.00
ATOM	436	N	GLY			80.558	57.601	9.698	1.00 20.00
ATOM	437	CA	GLY			80.674	57.344	11.112	1.00 20.00
ATOM	438	C	GLY			79.343	57.592	11.791	1.00 20.00
ATOM	439	ō	GLY			78.672	56.648	12.170	1.00 20.00
ATOM	441	N	GLU			78.958	58.864	11.901	1.00 20.00
ATOM	442	CA	GLU			77.690	59.258	12.529	1.00 20.00
ATOM	443	C	GLU			76.698	58.115	12.297	1.00 20.00
ATOM	444	0	GLU			76.096	57.579	13.241	1.00 20.00
ATOM	445	CB	GLU					11.939	1.00 20.00
ATOM	446	CG	GLU			77.178 76.581	60.602 60.552	10.530	1.00 20.00
ATOM	447	CD	GLU						
ATOM	448	OE1	GLU			75.027 74.433	60.750 60.770	9.383	1.00 20.00
		OE2							
ATOM	449		GLU			74.405	60.881	11.596	1.00 20.00
ATOM	451	N	LEU			76.545	57.753	11.028	1.00 20.00
MOTA	452	CA	LEU			75.726	56.633	10.649	1.00 20.00
ATOM	453	С	LEU			76.593	55.505	11.273	1.00 20.00
ATOM	454	0	LEU			76.715	55.463	12.500	1.00 20.00
MOTA	455	CB	LEU			75.658	56.527	9.101	1.00 20.00
ATOM	457	N	GLU			77.195	54.620	10.458	1.00 20.00
MOTA	458	CA	GLU			78.069	53.539	10.975	1.00 20.00
MOTA	459	C	GLU			77.903	53.535	12.468	1.00 20.00
ATOM	460	0	GLU			76.948	52.968	12.998	1.00 20.00
MOTA	461	CB	GLU			79.526	53.831	10.639	1.00 20.00
ATOM	463	N	VAL			78.838	54.222	13.116	1.00 20.00
ATOM	464	CA	VAL			78.847	54.419	14.567	1.00 20.00
ATOM	465	C	VAL			77.770	53.658	15.342	1.00 20.00
ATOM	466	0	VAL			78.065	52.892	16.266	1.00 20.00
ATOM	467	CB	VAL			78.756	55.961	14.897	1.00 20.00
ATOM	469	N	LEU			76.520	53.887	14.966	1.00 20.00
MOTA	470	CA	LEU			75.408	53.237	15.630	1.00 20.00
MOTA	471	C	LEU		876	75.957	51.873	16.004	1.00 20.00
MOTA	472	0			876	75.727	51.387	17.126	1.00 20.00
MOTA	473	CB	LEU	A	876	74.208	53.192	14.684	1.00 20.00
ATOM	474	CG	LEU		876	73.839	54.662	14.399	1.00 20.00
MOTA	475	CD1	LEU	Α	876	73.193	54.792	13.056	1.00 20.00
ATOM	476	CD2	LEU	Α	876	72.942	55.198	15.481	1.00 20.00
ATOM	478	N	CYS	A	877	76.744	51.320	15.071	1.00 20.00
MOTA	479	CA	CYS	Α	877	77.459	50.027	15.212	1.00 20.00
MOTA	480	C	CYS	Α	877	77.658	49.645	16.685	1.00 20.00
ATOM	481	0	CYS	A	877	77.099	48.656	17.205	1.00 20.00
ATOM	482	CB	CYS	A	877	78.855	50.137	14.546	1.00 20.00
ATOM	483	SG	CYS	Α		79.630	51.894	14.438	1.00 20.00
ATOM	485	N	LYS			78.447	50.496	17.337	1.00 20.00
MOTA	486	CA	LYS	A	878	78.789	50.363	18.762	1.00 20.00
ATOM	487	C	LYS	Α	878	77.629	49.811	19.612	1.00 20.00
ATOM	488	0	LYS	Α	878	77.847	49.438	20.805	1.00 20.00

MOTA	489	CB	LYS	А	878	79.260	51.733	19.351	1.00 20.00
ATOM	490	CG	LYS			80.718	52.114	19.017	1.00 20.00
ATOM	491	CD			878	81.321	52.986	20.114	1.00 20.00
ATOM	492	CE			878	81.612	54.418	19.609	1.00 20.00
ATOM	493	NZ			878	81.754	54.601	18.098	1.00 20.00
ATOM	498	N	LEU		879	76.427	49.792	19.000	1.00 20.00
ATOM	499	CA			879	75.203	49.320	19.634	1.00 20.00
ATOM	500	C			879	74.179	49.039	18.584	1.00 20.00
ATOM	501	ō	LEU		879	73.068	49.544	18.652	1.00 20.00
ATOM	502	CB	LEU		879	74.620	50.336	20.651	1.00 20.00
ATOM	503	CG	LEU			74.799	51.863	20.603	1.00 20.00
ATOM	504	CD1	LEU			75.966	52.280	21.461	1.00 20.00
ATOM	505	CD2	LEU			75.015	52.321	19.200	1.00 20.00
ATOM	507	N	GLY			74.546	48.227	17.597	1.00 20.00
ATOM	508	CA	GLY			73.551	47.899	16.578	1.00 20.00
ATOM	509	C	GLY			72.345	47.314	17.330	1.00 20.00
ATOM	510	o	GLY			71.296	47.906	17.464	1.00 20.00
ATOM	512	N	HIS			72.545	46.101	17.820	1.00 20.00
ATOM	513	CA	HIS			71.575	45.353	18.572	1.00 20.00
ATOM	514	C	HIS			71.402		19.917	1.00 20.00
ATOM	515	0	HIS			71.758	46.024 47.183	20.106	1.00 20.00
ATOM	516	CB	HIS			72.059	43.906	18.744	1.00 20.00
ATOM	517	CG	HIS			71.015	42.958	19.255	1.00 20.00
ATOM	518		HIS		881				
ATOM	519	CD2	HIS			69.952	42.520	18.485	1.00 20.00
ATOM	520	CE1				70.877	42.349	20.464	1.00 20.00
ATOM		NE2	HIS			69.207	41.691	19.197	1.00 20.00
ATOM	521 525	NE2	HIS			69.746	41.566	20.402	1.00 20.00
ATOM	526	CA				70.870	45.217	20.817	1.00 20.00
ATOM		C	HIS			70.420	45.429	22.177	1.00 20.00
ATOM	527 528	0	HIS			68.935	45.241	21.763	1.00 20.00
ATOM		CB	HIS			68.440	45.758	20.724	1.00 20.00
ATOM	529					70.704	46.804	22.806	1.00 20.00
	530	CG	HIS			70.491	46.812	24.295	1.00 20.00
ATOM	531	ND1				69.252	46.654	24.868	1.00 20.00
ATOM	532	CD2	HIS			71.365	46.839	25.325	1.00 20.00
ATOM	533	CEI	HIS			69.373	46.579	26.183	1.00 20.00
ATOM	534	NE2	HIS			70.645	46.686	26.486	1.00 20.00
ATOM ATOM	538	N	PRO			68.210	44.463	22.547	1.00 20.00
	539	CA	PRO			66.820	44.253	22.152	1.00 20.00
ATOM	540	C	PRO			66.019	45.510	22.212	1.00 20.00
ATOM	541	0	PRO			65.100	45.685	21.439	1.00 20.00
ATOM	542	CB	PRO			66.309	43.176	23.108	1.00 20.00
ATOM	543	CG	PRO			67.285	43.129	24.211	1.00 20.00
ATOM	544	CD	PRO			68.560	43.829	23.819	1.00 20.00
ATOM	545	N	ASN			66.414	46.408	23.098	1.00 20.00
MOTA	546	CA	ASN			65.710	47.650	23.263	1.00 20.00
ATOM	547	C	ASN			66.169	48.856	22.439	1.00 20.00
MOTA	548	0	ASN			65.801	49.977	22.723	1.00 20.00
MOTA	549	CB	ASN			65.672	47.898	24.749	1.00 20.00
ATOM	550	CG	ASN			65.444	46.594	25.498	1.00 20.00
ATOM	551	OD1	ASN			65.835	46.388	26.649	1.00 20.00
MOTA	552	ND2	ASN			64.817	45.687	24.802	1.00 20.00
MOTA	556	N			885	66.917	48.603	21.375	1.00 20.00
MOTA	557	CA			885	67.391	49.655	20.482	1.00 20.00
ATOM	558	C	ILE		885	67.205	49.202	19.020	1.00 20.00
ATOM	559	0			885	67.847	48.251	18.589	1.00 20.00
ATOM	560	CB	ILE	Α	885	68.930	50.021	20.761	1.00 20.00

MOTA	561	CG1	ILE .	A	885	69.032	50.962	21.954	1.00 20.00	
ATOM	562	CG2	ILE .	Α	885	69.529	50.830	19.639	1.00 20.00	
MOTA	563	CD1	ILE .	Α	885	70.397	51.213	22.385	1.00 20.00	
ATOM	565	N	ILE .	A	886	66.325	49.886	18.282	1.00 20.00	
ATOM	566	CA	ILE .			66.030	49.608	16.871	1.00 20.00	
ATOM	567	С	ILE :		886	67.338	49.271	16.206	1.00 20.00	
ATOM	568	0			886	68.363	49.491	16.788	1.00 20.00	
ATOM	569	CB	ILE :	Α	886	65.331	50.854	16.183	1.00 20.00	
ATOM	570	CG1	ILE :	Α	886	63.806	50.758	16.349	1.00 20.00	
ATOM	571	CG2	ILE :			65.568	50.868	14.691	1.00 20.00	
ATOM	572	CD1			886	63.134	49.624	15.492	1.00 20.00	
ATOM	574	N	ASN :	A	887	67.347	48.757	14.990	1.00 20.00	
ATOM	575	CA	ASN .	А	887	68.628	48.381	14.442	1.00 20.00	
ATOM	576	C			887	68.846	48.692	13.013	1.00 20.00	
ATOM	577	0	ASN .		887	67.889	48.902	12.273	1.00 20.00	
ATOM	578	CB	ASN .		887	68.827	46.892	14.597	1.00 20.00	
ATOM	579	CG	ASN .	A	887	70.276	46.512	14.731	1.00 20.00	
ATOM	580	OD1	ASN .			71.015	46.382	13.725	1.00 20.00	
ATOM	581	ND2	ASN			70.702	46.315	15.979	1.00 20.00	
ATOM	585	N	LEU .			70.118	48.684	12.604	1.00 20.00	
ATOM	586	CA	LEU .			70.417	48.950	11.203	1.00 20.00	
ATOM	587	С	LEU .			70.410	47.641	10.469	1.00 20.00	
ATOM	588	ō	LEU .		888	71.128	46.705	10.852	1.00 20.00	
ATOM	589	CB	LEU			71.799	49.586	11.000	1.00 20.00	
ATOM	590	CG	LEU		888	72.125	49.333	9.517	1.00 20.00	
ATOM	591	CD1	LEU			71.290	50.292	8.712	1.00 20.00	
ATOM	592	CD2	LEU :		888	73.594	49.451	9.207	1.00 20.00	
ATOM	594	N	LEU :		889	69.617	47.531	9.425	1.00 20.00	
ATOM	595	CA	LEU .			69.676	46.284	8.712	1.00 20.00	
ATOM	596	C	LEU .		889	70.630	46.494	7.567	1.00 20.00	
ATOM	597	0	LEU .			71.830	46.369	7.746	1.00 20.00	
ATOM	598	CB	LEU		889	68.310	45.906	8.247	1.00 20.00	
ATOM	599	CG	LEU .			67.451	45.554	9.465	1.00 20.00	
ATOM	600	CD1	LEU .			66.321	44.719	8.913	1.00 20.00	
ATOM	601	CD2	LEU		889	68.201	44.811	10.568	1.00 20.00	
ATOM	603	N			890	70.114	46.838	6.396	1.00 20.00	
ATOM	604	CA	GLY .			70.971	47.127	5.254	1.00 20.00	
ATOM	605	C	GLY :			71.310	48.613	5.048	1.00 20.00	
ATOM	606	ō	GLY .			71.237	49.441	5.951	1.00 20.00	
ATOM	608	N	ALA .			71.684	48.930	3.819	1.00 20.00	
ATOM	609	CA	ALA.			72.084	50.262	3.393	1.00 20.00	
MOTA	610	C	ALA.			72.437	50.082	1.907	1.00 20.00	
ATOM	611	ō	ALA.			72.299	48.965	1.361	1.00 20.00	
ATOM	612	CB	ALA.			73.296	50.706	4.166	1.00 20.00	
ATOM	614	N			892	72.908	51.153	1.262	1.00 20.00	
ATOM	615	CA	CYS .			73.258	51.085	-0.166	1.00 20.00	
ATOM	616	C			892	73.174	52.468	-0.776	1.00 20.00	
ATOM	617	ō	CYS			72.263	53.232	-0.453	1.00 20.00	
ATOM	618	CB		A	892	72.277	50.171	-0.952	1.00 20.00	
ATOM	619	SG		A	892	72.953	48.465	-1.345	1.00 20.00	
ATOM	621	N	GLU .		893	74.089	52.785	-1.680	1.00 20.00	
ATOM	622	CA	GLU		893	74.062	54.101	-2.298	1.00 20.00	
ATOM	623	C	GLU .		893	73.386	54.004	-3.637	1.00 20.00	
ATOM	624	ŏ	GLU		893	73.956	53.509	-4.616	1.00 20.00	
ATOM	625	CB	GLU .		893	75.483	54.655	-2.463	1.00 20.00	
ATOM	626	CG	GLU		893	76.613	53.751	-1.900	1.00 20.00	
ATOM	627	CD	GLU		893	77.227	52.860	-2.966	1.00 20.00	
			220				-2.000	2.500		

MOTA	628		GLU			76.831	52.998	-4.151	1.00 20.00
ATOM	629	OE2	GLU		893	78.105	52.033	~2.612	1.00 20.00
ATOM	631	N	HIS		894	72.140	54.427	-3.684	1.00 20.00
MOTA	632	CA	HIS		894	71.437	54.382	-4.949	1.00 20.00
MOTA	633	C	HIS		894	71.690	55.786	-5.419	1.00 20.00
ATOM	634	0	HIS	Α	894	71.305	56.755	-4.750	1.00 20.00
MOTA	635	CB	HIS	А	894	69.937	54.149	-4.753	1.00 20.00
ATOM	636	CG	HIS	A	894	69.133	54.328	-6.003	1.00 20.00
MOTA	637	ND1	HIS	Α	894	67.767	54.494	-5.990	1.00 20.00
ATOM	638	CD2	HIS	A	894	69.510	54.413	-7.301	1.00 20.00
ATOM	639	CE1	HIS	A	894	67.332	54.680	-7.223	1.00 20.00
ATOM	640	NE2	HIS	А	894	68.369	54.634	-8.037	1.00 20.00
MOTA	644	N	ARG	Α	895	72.366	55.873	-6.556	1.00 20.00
ATOM	645	CA	ARG	A	895	72.768	57.132	-7.151	1.00 20.00
ATOM	646	C	ARG	A	895	71.873	58.311	-6.767	1.00 20.00
ATOM	647	0	ARG	Α	895	70.654	58.317	-7.001	1.00 20.00
ATOM	648	CB	ARG		895	72.910	56.904	-8.643	1.00 20.00
ATOM	649	CG	ARG			73.918	55.775	-8.856	1.00 20.00
ATOM	650	CD	ARG		895	73.482	54.825	-9.910	1.00 20.00
ATOM	651	NE	ARG		895	74.001		-11.176	1.00 20.00
ATOM	652	CZ	ARG		895	73.609	54.881	-12.370	1.00 20.00
ATOM	653		ARG		895	72.657	53.926	-12.469	1.00 20.00
ATOM	654	NH2	ARG		895	74.183		-13.460	1.00 20.00
ATOM	661	N	GLY			72.510	59.315	-6.177	1.00 20.00
ATOM	662	CA	GLY			71.781	60.441	-5.654	1.00 20.00
ATOM	663	C	GLY			71.761	60.040	-4.207	1.00 20.00
ATOM	664	0	GLY			72.194	58.860	-3.967	1.00 20.00
ATOM	666	N	TYR		897	71.919	60.962	-3.254	1.00 20.00
ATOM									
	667	CA	TYR		897	72.066	60.604	-1.839	1.00 20.00
ATOM	668	C	TYR		897	71.643	59.133	-1.531	1.00 20.00
ATOM	669	0	TYR		897	70.959	58.507	-2.336	1.00 20.00
ATOM	670	CB	TYR			71.195	61.548	-1.039	1.00 20.00
MOTA	671	CG	TYR		897	71.828	62.224	0.128	1.00 20.00
ATOM	672	CD1	TYR		897	73.097	62.810	0.030	1.00 20.00
ATOM	673	CD2	TYR		897	71.116	62.358	1.321	1.00 20.00
ATOM	674	CE1	TYR		897	73.638	63.526	1.108	1.00 20.00
ATOM	675	CE2	TYR		897	71.641	63.069	2.402	1.00 20.00
ATOM	676	CZ	TYR		897	72.894	63.650	2.290	1.00 20.00
MOTA	677	OH	TYR			73.381	64.361	3.369	1.00 20.00
MOTA	680	N	LEU	А	898	72.001	58.564	-0.369	1.00 20.00
ATOM	681	CA	LEU			71.571	57.163	-0.196	1.00 20.00
ATOM	682	C	LEU			71.131	56.437	1.099	1.00 20.00
MOTA	683	0	LEU	Α	898	71.759	56.483	2.161	1.00 20.00
ATOM	684	CB	LEU	Α	898	72.542	56.240	-0.990	1.00 20.00
ATOM	686	N	TYR	А	899	70.041	55.704	0.830	1.00 20.00
MOTA	687	CA	TYR	A	899	69.162	54.833	1.624	1.00 20.00
MOTA	688	C	TYR	Α	899	69.544	53.804	2.665	1.00 20.00
ATOM	689	0	TYR	Α	899	70.411	52.969	2.445	1.00 20.00
ATOM	690	CB	TYR	Α	899	68.268	54.076	0.657	1.00 20.00
ATOM	691	CG	TYR		899	67.523	54.943	-0.339	1.00 20.00
ATOM	692	CD1	TYR		899	68.208	55.776	-1.209	1.00 20.00
ATOM	693	CD2	TYR			66.163	54.790	-0.522	1.00 20.00
ATOM	694	CE1	TYR		899	67.574	56.407	-2.238	1.00 20.00
ATOM	695	CE2	TYR		899	65.514	55.429	-1.564	1.00 20.00
ATOM	696	CZ	TYR		899	66.225	56.235	-2.431	1.00 20.00
ATOM	697	OH	TYR			65.602	56.841	-3.510	1.00 20.00
ATOM	700	N	LEU			68.814	53.814	3.775	1.00 20.00
				_	- 50	50.014	23.014	3.775	2.00 20.00

Inventors:

Title: Method of Identifying Inhibitors of TIE-2 Nancy J. Bump et al.

ATOM 701 CA LEU A 900 69.047 52.841 4.845 1.00 20.00 ATOM 702 C LEU A 900 67.805 51.988 5.149 1.00 20.00 703 O MOTA LEU A 900 66.645 52.459 5.109 1.00 20.00 ATOM 704 CB LEU A 900 69.455 53.522 6.147 1.00 20.00 705 CG LEU A 900 MOTA 70.810 54.184 6.259 1.00 20.00 ATOM 706 CD1 LEU A 900 71.404 54.368 4.864 1.00 20.00 707 CD2 LEU A 900 ATOM 70.624 55.498 7.033 1.00 20.00 MOTA 709 N ALA A 901 68.083 50.739 5.495 1.00 20.00 ATOM 710 CA ALA A 901 67.043 49.813 5.811 1.00 20.00 67.113 49.495 7.275 1.00 20.00 67.828 48.577 7.670 1.00 20.00 67.221 48.564 5.003 1.00 20.00 66.372 50.260 8.078 1.00 20.00 65.367 48.888 9.812 1.00 20.00 65.367 48.888 9.812 1.00 20.00 65.801 51.315 10.167 1.00 20.00 65.802 51.305 10.058 10.058 10.00 20.00 65.308 51.006 11.556 1.00 20.00 65.308 51.006 11.556 1.00 20.00 67.878 52.583 11.280 1.00 20.00 67.878 52.583 11.280 1.00 20.00 64.435 47.350 11.465 1.00 20.00 64.435 47.350 11.465 1.00 20.00 62.997 47.870 11.652 1.00 20.00 67.043 49.813 5.811 1.00 20.00 ATOM 711 C ALA A 901 ATOM 712 O ALA A 901 ATOM 713 CB ALA A 901 ATOM 715 N ILE A 902 ATOM 716 CA ILE A 902 ATOM 717 C ILE A 902 ATOM 718 0 ILE A 902 719 CB ILE A 902 ATOM ATOM 720 CG1 ILE A 902 721 CG1 ILE A 902
721 CG2 ILE A 902
722 CD1 ILE A 902
724 N GLU A 903
725 CA GLU A 903
726 C GLU A 903 ATOM ATOM MOTA ATOM ATOM 62.997 47.870 11.692 1.00 20.00 ATOM 727 O GLU A 903 62.713 48.559 12.662 1.00 20.00 ATOM 728 CB GLU A 903 64.973 46.703 12.746 1.00 20.00 MOTA 729 CG GLU A 903 63.985 45.965 13.580 1.00 20.00 ATOM 730 CD GLU A 903 64.471 45.766 15.006 1.00 20.00 ATOM 731 OE1 GLU A 903 63.971 44.875 15.725 1.00 20.00 65.365 46.509 15.425 1.00 20.00 62.115 47.514 10.767 1.00 20.00 60.707 47.846 10.758 1.00 20.00 ATOM 732 OE2 GLU A 903 1 ATOM 734 N TYR A 904 ATOM 735 CA TYR A 904 ATOM 736 C TYR A 904 59.985 47.328 11.989 1.00 20.00 ATOM 737 O TYR A 904 60.054 46.149 12.240 1.00 20.00 60.078 47.204 9.521 1.00 20.00 738 CB TYR A 904 ATOM 739 CG TYR A 904 ATOM 58.553 47.146 9.537 1.00 20.00 740 CD1 TYR A 904 ATOM 57.795 48.150 8.920 1.00 20.00 ATOM 741 CD2 TYR A 904 57.868 46.125 10.188 1.00 20.00 ATOM 742 CE1 TYR A 904 56.420 48.136 8.955 1.00 20.00 743 CE2 TYR A 904 ATOM 56.498 46.115 10.223 1.00 20.00 ATOM 744 CZ TYR A 904 55.779 47.128 9.602 1.00 20.00 ATOM 745 OH TYR A 904 54.405 47.149 9.622 1.00 20.00 ATOM 748 N ALA A 905 59.270 48.183 12.727 1.00 20.00 ATOM 749 CA ALA A 905 58.503 47.772 13.931 1.00 20.00 MOTA 750 C ALA A 905 56.987 47.506 13.620 1.00 20.00 ATOM 751 0 ALA A 905 56.395 48.128 12.744 1.00 20.00 ATOM 752 CB ALA A 905 58.649 48.816 14.976 1.00 20.00 ATOM 754 N PRO A 906 56.341 46.572 14.317 1.00 20.00 ATOM 755 CA PRO A 906 54.949 46.394 13.918 1.00 20.00 ATOM 756 C PRO A 906 53.803 46.643 14.902 1.00 20.00 ATOM 757 O PRO A 906 52.992 45.748 15.150 1.00 20.00 ATOM 54.958 44.937 13.468 1.00 20.00 758 CB PRO A 906 ATOM 759 CG PRO A 906 55.981 44.280 14.584 1.00 20.00 760 CD PRO A 906 ATOM 56.719 45.482 15.227 1.00 20.00 MOTA 761 N HIS A 907 53.729 47.841 15.450 1.00 20.00 52.655 48.251 16.349 1.00 20.00 52.966 49.700 16.468 1.00 20.00 52.865 50.262 17.534 1.00 20.00 ATOM 762 CA HIS A 907 ATOM 763 C HIS A 907 ATOM 764 O HIS A 907

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Docket/App No.: 2079.1037-001

Title: Method of Identifying Inhibitors of TIE-2 Nancy J. Bump et al. Inventors:

ATOM	765	СВ	HIS	Δ	907	52.745	47.577	17.714	1.00 20.00
ATOM	766	CG		Α	907	52.656	46.090	17.650	1.00 20.00
ATOM	767			Α	907	53.753	45.272	17.799	1.00 20.00
ATOM	768	CD2		A	907	51.622	45.274	17.350	1.00 20.00
ATOM	769	CE1		Α	907	53.404	44.018	17.593	1.00 20.00
ATOM	770	NE2	HIS	Α	907	52.116	43.993	17.318	1.00 20.00
ATOM	774	N	GLY	А	908	53.411	50.280	15.365	1.00 20.00
ATOM	775	CA	GLY	Α	908	53.733	51.676	15.348	1.00 20.00
MOTA	776	C	GLY	Α	908	54.622	52.111	16.486	1.00 20.00
ATOM	777	0	GLY	Α	908	55.525	51.381	16.887	1.00 20.00
ATOM	779	1/1	ASN	Α	909	54.338	53.284	17.054	1.00 20.00
ATOM	780	CA	ASN	Α	909	55.183	53.854	18.094	1.00 20.00
ATOM	781	C	ASN	A	909	54.590	53.912	19.463	1.00 20.00
MOTA	782	0	ASN	A	909	53.409	54.064	19.616	1.00 20.00
MOTA	783	CB	ASN	Α	909	55.545	55.270	17.672	1.00 20.00
MOTA	784	CG	ASN	Α	909	54.346	56.201	17.669	1.00 20.00
MOTA	785	OD1	ASN	Α	909	54.409	57.315	17.192	1.00 20.00
ATOM	786		ASN			53.260	55.738	18.210	1.00 20.00
MOTA	790	N	LEU		910	55.414	53.878	20.482	1.00 20.00
ATOM	791	CA	LEU		910	54.872	53.913	21.808	1.00 20.00
MOTA	792	C	LEU		910	53.703	54.890	21.927	1.00 20.00
MOTA	793	0	LEU			52.760	54.647	22.669	1.00 20.00
ATOM	794	CB	LEU			55.949	54.257	22.797	1.00 20.00
ATOM	795	CG	LEU		910	55.456	54.079	24.220	1.00 20.00
MOTA	796	CD1	LEU			54.921	52.676	24.488	1.00 20.00
ATOM	797	CD2	LEU		910	56.617	54.427	25.133	1.00 20.00
MOTA	799	N	LEU		911	53.725	56.005	21.219	1.00 20.00
ATOM	800	CA	LEU		911	52.578	56.862	21.381	1.00 20.00
ATOM	801	C	LEU			51.408	56.200	20.656	1.00 20.00
ATOM	802	0	LEU		911	50.700	55.442	21.275	1.00 20.00
ATOM	803	CB	LEU		911	52.820	58.302	20.863	1.00 20.00
ATOM ATOM	804 805	CG	LEU			51.958	59.498	21.354	1.00 20.00
ATOM	806	CD1	LEU			51.738	59.517	22.855	1.00 20.00
ATOM	808	N N	LEU ASP		911	52.645	60.737	20.917	1.00 20.00
ATOM	809	CA			912	51.219	56.459	19.371	1.00 20.00
ATOM	810	C			912	50.117 49.646	55.895	18.642	1.00 20.00
ATOM	811	0			912	48.468	54.540	19.121	1.00 20.00
ATOM	812	CB			912	50.461	54.225 55.849	19.083 17.181	1.00 20.00
ATOM	813	CG			912	50.214	57.151	16.498	1.00 20.00
ATOM	814				912	50.507	57.259	15.304	1.00 20.00
ATOM	815		ASP		912	49.725	58.089	17.141	1.00 20.00
ATOM	817	N			913	50.572	53.703	19.562	1.00 20.00
ATOM	818	CA	PHE		913	50.168	52.405	20.098	1.00 20.00
ATOM	819	c	PHE			49.397	52.903	21.287	1.00 20.00
ATOM	820	ō			913	48.236	53.231	21.164	1.00 20.00
MOTA	821	CB	PHE			51.355	51.585	20.547	1.00 20.00
ATOM	822	CG	PHE		913	51.010	50.182	20.847	1.00 20.00
ATOM	823	CD1			913	50.511	49.365	19.866	1.00 20.00
ATOM	824	CD2			913	51.133	49.688	22.122	1.00 20.00
ATOM	825	CE1			913	50.141	48.088	20.152	1.00 20.00
MOTA	826	CE2			913	50.760	48.418	22.407	1.00 20.00
ATOM	827	CZ	PHE	Α	913	50.263	47.619	21.418	1.00 20.00
MOTA	829	N	LEU	Α	914	50.059	53.031	22.416	1.00 20.00
MOTA	830	CA	LEU	Α	914	49.400	53.584	23.572	1.00 20.00
ATOM	831	C	LEU		914	48.080	54.304	23.288	1.00 20.00
MOTA	832	0	LEU	Α	914	47.102	54.093	23.985	1.00 20.00

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Title: Method of Identifying Inhibitors of TIE-2 Inventors: Nancy J. Bump *et al.*

ATOM	833	СВ	ז דים ז	7	914	E0 242	54 540	04.044		00.00
ATOM	834	CG			914	50.342 51.146	54.549	24.244		20.00
ATOM	835	CD1			914	52.130	53.995 55.080	25.410 25.953	1.00	20.00
ATOM	836		LEU			50.142				
ATOM	838	N N	ARG		915	48.006	53.501 55.139	26.466		20.00
ATOM	839	CA			915			22.265		
ATOM	840	C			915	46.736	55.841	22.041	1.00	
ATOM	841	0			915	45.650	54.970	21.526	1.00	
ATOM	842	CB			915	44.569	54.984	22.054	1.00	20.00
ATOM						46.896	57.078	21.141	1.00	20.00
ATOM	843 844	CG			915	46.687	58.379	21.885	1:00	
ATOM					915	47.528	59.415	21.256	1.00	
ATOM	845 846	NE CZ			915	48.215	60.347	22.169	1.00	20.00
ATOM			ARG			48.763	61.482	21.760	1.00	
ATOM	847 848		ARG		915	48.709	61.835	20.494	1.00	
ATOM			ARG			49.383	62.240	22.602	1.00	20.00
ATOM	855	N	LYS		916	45.943	54.219	20.485	1.00	20.00
	856	CA	LYS			45.019	53.242	19.890	1.00	
ATOM	857	C	LYS		916	44.681	52.169	20.920	1.00	20.00
ATOM	858	0	LYS			44.275	51.109	20.561	1.00	20.00
ATOM	859	CB			916	45.714	52.563	18.676	1.00	
ATOM	860	CG	LYS			45.988	51.000	18.704	1.00	
ATOM	861	CD	LYS			46.802	50.408	19.888	1.00	
ATOM	862	CE	LYS			46.861	48.841	19.822	1.00	20.00
ATOM	863	NZ	LYS			46.225	47.974	20.937	1.00	20.00
ATOM	868	N	SER			44.851	52.438	22.196	1.00	20.00
ATOM	869	CA	SER			44.597	51.466	23.204	1.00	
ATOM	870	С	SER			43.641	52.011	24.233	1.00	20.00
ATOM	871	0	SER			43.501	51.444	25.330	1.00	20.00
ATOM	872	CB	SER			45.891	51.147	23.883	1.00	
ATOM	873	OG	SER			45.843	51.568	25.227		20.00
ATOM	876	N	ARG		918	43.014	53.138	23.902	1.00	20.00
ATOM	877	CA	ARG		918	42.041	53.822	24.775	1.00	20.00
ATOM	878	C	ARG		918	40.816	53.359	24.014	1.00	20.00
ATOM	879	0	ARG			40.523	53.883	22.951	1.00	20.00
ATOM	880	CB	ARG		918	42.260	55.365	24.669	1.00	20.00
ATOM	881	CG	ARG			43.138	56.036	25.794	1.00	20.00
MOTA	882	CD	ARG		918	43.547	57.502	25.488	1.00	20.00
MOTA	883	NE	ARG			44.494	57.982	26.502	1.00	20.00
ATOM	884	CZ	ARG			44.777	59.260	26.795	1.00	20.00
ATOM	885		ARG			44.211	60.289	26.165	1.00	20.00
ATOM	886	NH2	ARG			45.625	59.523	27.777	1.00	20.00
ATOM	8 93	N	VAL			40.135	52.333	24.507	1.00	20.00
MOTA	894	CA	VAL			39.009	51.770	23.757	1.00	20.00
ATOM	895	C	VAL			37.733	52.382	24.202	1.00	20.00
ATOM	896	0	VAL			36.750	52.427	23.450	1.00	20.00
ATOM	897	CB	VAL			38.925	50.198	23.861	1.00	20.00
MOTA	898	CG1	VAL	Α	919	40.218	49.603	23.459	1.00	20.00
ATOM	899	CG2	VAL	Α	919	38.550	49.746	25.275	1.00	20.00
MOTA	901	N	LEU		920	37.736	52.861	25.432	1.00	20.00
ATOM	902	CA	LEU	Α	920	36.569	53.542	25.895	1.00	20.00
ATOM	903	C	LEU	Α	920	36.303	54.630	24.864	1.00	20.00
MOTA	904	0	LEU	Α	920	35.276	55.259	24.906	1.00	20.00
ATOM	905	CB	LEU	Α	920	36.815	54.146	27.236	1.00	20.00
MOTA	906	CG	LEU	Α	920	35.641	54.652	28.011	1.00	20.00
MOTA	907	CD1	LEU	Α	920	35.060	53.567	28.831	1.00	20.00
ATOM	908	CD2	LEU	Α	920	36.155	55.768	28.901	1.00	20.00
ATOM	910	N	GLU	Α	921	37.224	54.824	23.926	1.00	20.00

Title: Method of Identifying Inhibitors of TIE-2 Inventors: Nancy J. Bump et al.

ATOM	911	CA	GLU	Α	921	37.081	55.783	22.850	1.00	20.00
ATOM	912	C	GLU	Α	921	37.413	55.109	21.541	1.00	20.00
ATOM	913	ō	GLU			37.205	55.677	20.469		20.00
ATOM	914	CB	GLU			38.047	56.940	23.011		20.00
ATOM	915	CG	GLU			38.258	57.743	21.736		20.00
ATOM	916	CD	GLU			39.404	58.696	21.848		20.00
	917		GLU			39.875	58.879	22.982		20.00
MOTA		OE1								
ATOM	918		GLU			39.836	59.261	20.825		20.00
ATOM	920	N	THR			37.936	53.893	21.615		20.00
ATOM	921	CA	THR			38.309	53.178	20.413		20.00
ATOM	922	С	THR			37.429	51.960	20.078		20.00
ATOM	923	0	THR			37.502	51.387	18.963		20.00
ATOM	924	CB	THR			39.742	52.728	20.559		20.00
ATOM	925		THR			40.441	53.058	19.366		20.00
ATOM	926		THR			39.824	51.214	20.816		20.00
ATOM	929	N	ASP			36.617	51.575	21.074	1.00	20.00
MOTA	930	CA	ASP	Α	923	35.712	50.423	21.026	1.00	20.00
MOTA	931	C	ASP	A	923	34.972	50.387	22.350	1.00	20.00
ATOM	932	0	ASP	Α	923	35.259	49.550	23.203	1.00	20.00
ATOM	933	CB	ASP	А	923	36.494	49.119	20.905	1.00	20.00
ATOM	934	CG	ASP	A	923	35.879	48.142	19.909	1.00	20.00
ATOM	935	OD1	ASP	Α	923	35.624	48.553	18.745	1.00	20.00
MOTA	936	OD2	ASP	А	923	35.669	46.956	20.271	1.00	20.00
MOTA	938	N	PRO	Α	924	34.042	51.323	22.577	1.00	20.00
ATOM	939	CA	PRO			33.362	51.211	23.874		20.00
ATOM	940	C	PRO	А	924	32.544	49.923	24.176	1.00	20.00
ATOM	941	0	PRO			32.172	49.720	25.342	1.00	20.00
ATOM	942	CB	PRO			32.540	52.506	23.953		20.00
ATOM	943	CG			924	33.214	53.417	22.960		20.00
ATOM	944	CD	PRO			33.600	52.512	21.841		20.00
ATOM	945	N	ALA			32.276	49.078	23.156		20.00
ATOM	946	CA	ALA			31.551	47.770	23.326		20.00
ATOM	947	C	ALA			32.438	46.878	24.193		20.00
ATOM	948	o	ALA			32.016	46.274	25.190		20.00
ATOM	949	CB	ALA			31.328	47.103	21.992		20.00
ATOM	951	N	PHE			33.695	46.843	23.771		20.00
ATOM	952	CA	PHE			34.782	46.173	24.431	1.00	
ATOM	953	C	PHE			34.885	46.856	25.745		20.00
ATOM	954	0	PHE			34.896	46.269	26.772		20.00
ATOM	955	CB	PHE			36.058	46.460	23.667		20.00
ATOM	956	CG	PHE			37.046	45.347	23.693		20.00
ATOM	957		PHE				44.511	22.599		20.00
ATOM	958		PHE			37.164 37.810	45.127	24.825		20.00
ATOM	959		PHE					22.630		20.00
						38.003	43.493			
ATOM	960		PHE			38.661	44.107	24.881		20.00
ATOM	961	CZ	PHE			38.773	43.272	23.786		20.00
ATOM	963	N	ALA			35.024	48.154	25.681		20.00
ATOM	964	CA	ALA			35.084	48.926	26.885		20.00
ATOM	965	C	ALA			34.165	48.337	27.956		20.00
MOTA	966	0	ALA			34.695	47.721	28.843		20.00
MOTA	967	CB	ALA			34.717	50.348	26.587		20.00
MOTA	969	N	ILE			32.825	48.502	27.887		20.00
MOTA	970	CA	ILE			31.935	47.945	28.958		20.00
ATOM	971	C	ILE			31.760	46.437	29.001		20.00
ATOM	972	0	ILE			31.464	45.883	30.050		20.00
ATOM	973	CB			928	30.395	48.487	29.019		20.00
7 TOM	074	CCI	TITE	20	020	20 001	40 406	22 041	7 00	20 00

ATOM

974 CG1 ILE A 928

30.081 49.486 27.941 1.00 20.00

ATOM	975	CG2	ILE A	928	30.098	49.114	30.414	1.00 20.00
ATOM	976	CD1	ILE A		29.952	50.862	28.545	1.00 20.00
ATOM	978	N	ALA A		31.895	45.782	27.860	1.00 20.00
ATOM	979	CA	ALA A	929	31.747	44.356	27.867	1.00 20.00
ATOM	980	C	ALA A		32.803	43.844	28.804	1.00 20.00
ATOM	981	0	ALA A		32.525	43.055	29.667	1.00 20.00
ATOM	982	CB	ALA A		31.946	43.823	26.510	1.00 20.00
ATOM	984	N	ASN A		34.010	44.358	28.642	1.00 20.00
ATOM	985	CA	ASN A		35.181	44.009	29.429	1.00 20.00
ATOM	986	C	ASN A		35.448	44.882	30.665	1.00 20.00
ATOM	987	0	ASN A		36.191	44.496	31.566	1.00 20.00
ATOM	988	CB	ASN A		36.397	44.067	28.511	1.00 20.00
ATOM	989	CG	ASN A		36.628	42.771	27.745	1.00 20.00
ATOM	990		ASN A		37.333	41.876	28.220	1.00 20.00
ATOM	991		ASN A		36.046	42.671	26.547	1.00 20.00
ATOM	995	N	SER A		34.847	46.063	30.695	1.00 20.00
ATOM	996	CA	SER A		35.050	47.041	31.768	1.00 20.00
ATOM	997	C	SER A		36.531	47.527	31.922	1.00 20.00
ATOM	998	ō	SER A		37.074	47.556	33.020	1.00 20.00
ATOM	999	CB	SER A		34.541	46.453	33.084	1.00 20.00
ATOM	1000	OG	SER A		34.196	45.103	32.879	1.00 20.00
ATOM	1003	N	THR A		37.155	47.931	30.815	1.00 20.00
ATOM	1004	CA	THR A		38.545	48.392	30.821	1.00 20.00
ATOM	1005	C	THR A		38.800	49.536	29.872	1.00 20.00
ATOM	1006	ō	THR A		38.184	49.614	28.803	1.00 20.00
ATOM	1007	CB	THR A		39.525	47.299	30.451	1.00 20.00
ATOM	1008	OG1	THR A		38.971	46.481	29.417	1.00 20.00
ATOM	1009	CG2	THR A		39.832	46.479	31.663	1.00 20.00
ATOM	1012	N	ALA A		39.747	50.384	30.287	1.00 20.00
ATOM	1013	CA	ALA A		40.179	51.608	29.597	1.00 20.00
ATOM	1014	C	ALA A		41.172	51.417	28.495	1.00 20.00
ATOM	1015	ō	ALA A		41.155	52.134	27.513	1.00 20.00
ATOM	1016	CB	ALA A		40.778	52.547	30.597	1.00 20.00
ATOM	1018	N	SER A		42.086	50.480	28.709	1.00 20.00
ATOM	1019	CA	SER A		43.134	50.131	27.749	1.00 20.00
ATOM	1020	C	SER A		43.001	48.645	27.512	1.00 20.00
ATOM	1021	0	SER A		42.431	47.966	28.337	1.00 20.00
ATOM	1022	CB	SER A		44.511	50.396	28.374	1.00 20.00
ATOM	1023	OG	SER A		45.494	50.638	27.386	1.00 20.00
ATOM	1026	N	THR A		43,497	48.150	26.380	1.00 20.00
ATOM	1027	CA	THR A		43.529	46.701	26.144	1.00 20.00
ATOM	1028	C	THR A		44.801	46.297	26.814	1.00 20.00
ATOM	1029	ō	THR A		45.015	45.118	27.082	1.00 20.00
ATOM	1030	CB	THR A		43.768	46.312	24.783	1.00 20.00
ATOM	1031	OG1	THR A		44.892	47.021	24.325	1.00 20.00
ATOM	1032	CG2	THR A		42.571	46.583	23.961	1.00 20.00
ATOM	1035	N		936	45.640	47.301	27.070	1.00 20.00
ATOM	1036	CA	LEU A		46.897	47.138	27.735	1.00 20.00
ATOM	1037	C	LEU A		46.640	46.822	29.174	1.00 20.00
ATOM	1038	0	LEU A		45.579	47.010	29.666	1.00 20.00
ATOM	1039	CB	LEU A		47.699	48.413	27.635	1.00 20.00
ATOM	1040	CG	LEU A		47.921	49.086	26.273	1.00 20.00
ATOM	1041		LEU A		49.058	50.134	26.370	1.00 20.00
ATOM	1042		LEU A		48.250	48.029	25.238	1.00 20.00
ATOM	1044	N	SER A		47.652	46.322	29.841	1.00 20.00
ATOM	1045	CA	SER A		47.576	45.961	31.232	1.00 20.00
ATOM	1046	C	SER A		48.521	46.834	32.054	1.00 20.00
-	-	-					-2.054	

ATOM	1047	0	SER	A	937	49.291	47.608	31.519	1.00 20.00
ATOM	1048	CB	SER	А	937	47.988	44.501	31.384	1.00 20.00
ATOM	1049	OG	SER	A	937	48.630	44.257	32.628	1.00 20.00
MOTA	1052	N	SER	Α	938	48.458	46.695	33.365	1.00 20.00
ATOM	1053	CA	SER	А	938	49.319	47.433	34.239	1.00 20.00
ATOM	1054	С	SER	A	938	50.724	46.904	33.957	1.00 20.00
MOTA	1055	0	SER			51.686	47.668	33.847	1.00 20.00
ATOM	1056	CB	SER			48.900	47.177	35.683	1.00 20.00
MOTA	1057	OG	SER			50.012	47.071	36.555	1.00 20.00
ATOM	1060	N	GLN			50.849	45.587	33.812	1.00 20.00
ATOM	1061	CA	GLN			52.165	45.002	33.522	1.00 20.00
ATOM	1062	C	GLN			52.709	45.435	32.165	1.00 20.00
ATOM	1063	ō	GLN			53.831	45.917	32.073	1.00 20.00
ATOM	1064	CB	GLN		939	52.138	43,465	33.608	1.00 20.00
ATOM	1065	CG	GLN			52.298	42.909	35.046	1.00 20.00
ATOM	1066	CD	GLN			53.756	42.716	35.473	1.00 20.00
ATOM	1067	OEl	GLN			54.595	42.185	34.711	1.00 20.00
ATOM	1068	NE2	GLN			54.065	43.139	36.700	1.00 20.00
ATOM	1072	N	GLN			51.932	45.294	31.111	1.00 20.00
MOTA	1072	CA	GLN			52.445	45.696	29.813	1.00 20.00
ATOM	1074	c	GLN		940	53.040	47.092	29.913	1.00 20.00
ATOM	1075	0	GLN		940	53.944	47.477	29.163	1.00 20.00
ATOM	1076	CB	GLN			51.330	45.696	28.788	1.00 20.00
ATOM	1077	CG	GLN			51.695	46.374	27.506	1.00 20.00
ATOM	1077	CD	GLN			52.703		26.720	1.00 20.00
ATOM	1079	OE1	GLN		940	52.703	45.592 45.571	25.496	1.00 20.00
ATOM			GLN		940	53.591		27.418	1.00 20.00
	1080	NE2					44.934		1.00 20.00
MOTA	1084	N	LEU			52.523	47.832	30.887	
ATOM	1085	CA	LEU			52.918	49.212	31.110	1.00 20.00
MOTA	1086	C	LEU			54.285	49.397	31.744	1.00 20.00
ATOM	1087	0	LEU			55.074	50.181	31.231	1.00 20.00
ATOM	1088	CB	LEU		941	51.855	49.924	31.933	1.00 20.00
ATOM	1089	CG	LEU			50.700	50.500	31.161	1.00 20.00
ATOM	1090	CD1	LEU			50.187	51.653	31.924	1.00 20.00
ATOM	1091	CD2	LEU			51.139	50.904	29.785	1.00 20.00
ATOM	1093	N	LEU		942	54.571	48.720	32.848	1.00 20.00
ATOM	1094	CA	LEU			55.882	48.863	33.431	1.00 20.00
ATOM	1095	C	LEU			56.822	48.204	32.440	1.00 20.00
MOTA	1096	0	LEU			57.987	48.583	32.283	1.00 20.00
ATOM	1097	CB	LEU			55.955	48.147	34.756	1.00 20.00
MOTA	1098	CG	LEU		942	54.731	48.399	35.609	1.00 20.00
MOTA	1099	CD1	LEU			54.907	47.676	36.943	1.00 20.00
ATOM	1100	CD2			942	54.526	49.936	35.793	1.00 20.00
MOTA	1102	N	HIS			56.309	47.201	31.761	1.00 20.00
ATOM	1103	CA			943	57.127	46.548	30.800	1.00 20.00
ATOM	1104	C	HIS			57.754	47.596	29.894	1.00 20.00
ATOM	1105	0			943	58.969	47.781	29.936	1.00 20.00
ATOM	1106	CB	HIS		943	56.302	45.586	29.997	1.00 20.00
ATOM	1107	CG	HIS			56.549	44.159	30.350	1.00 20.00
MOTA	1108		HIS		943	56.709	43.732	31.649	1.00 20.00
MOTA	1109		HIS		943	56.634	43.054	29.582	1.00 20.00
MOTA	1110	CEl	HIS	Α	943	56.881	42.427	31.670	1.00 20.00
MOTA	1111	NE2	HIS	Α	943	56.841	41.994	30.427	1.00 20.00
MOTA	1115	N	PHE	Α	944	56.929	48.278	29.084	1.00 20.00
ATOM	1116	CA	PHE	A	944	57.396	49.327	28.162	1.00 20.00
ATOM	1117	C	PHE	Α	944	58.366	50.354	28.831	1.00 20.00
ATOM	1118	0	PHE	A	944	59.368	50.775	28.249	1.00 20.00

ATOM	1119	СВ	PHE	Δ	944	56.205	50.071	27.619	1.00 20.00
ATOM	1120	CG	PHE			55.484	49.372	26.515	1.00 20.00
ATOM	1121	CD1	PHE			54.116	49.207	26.572	1.00 20.00
ATOM	1122	CD2	PHE			56.130	49.020	25.368	1.00 20.00
MOTA	1123	CE1	PHE		944	53.432	48.727	25.515	1.00 20.00
ATOM	1124	CE2	PHE			55.433	48.534	24.300	1.00 20.00
ATOM	1125	CZ	PHE			54.096	48.393	24.375	1.00 20.00
ATOM	1127	N	ALA			58.055	50.749	30.057	1.00 20.00
ATOM	1128	CA	ALA			58.919	51.639	30.792	1.00 20.00
ATOM	1129	C	ALA			60.323	51.010	31.013	1.00 20.00
ATOM	1130	ō	ALA			61.349	51.690	30.906	1.00 20.00
MOTA	1131	CB	ALA			58.292	51.974	32.101	1.00 20.00
ATOM	1133	N	ALA	Α	946	60.373	49.710	31.297	1.00 20.00
MOTA	1134	CA	ALA			61.650	49.043	31.547	1.00 20.00
ATOM	1135	C	ALA			62.466	48.605	30.330	1.00 20.00
ATOM	1136	o	ALA			63.646	48.331	30.434	1.00 20.00
ATOM	1137	CB	ALA			61.418	47.872	32.429	1.00 20.00
MOTA	1139	N	ASP			61.823	48.486	29.188	1.00 20.00
ATOM	1140	CA	ASP	A	947	62.532	48.106	27.998	1.00 20.00
ATOM	1141	C	ASP			63.351	49.335	27.765	1.00 20.00
ATOM	1142	0	ASP			64.564	49.273	27.560	1.00 20.00
ATOM	1143	CB	ASP	Α	947	61.560	47.930	26.849	1.00 20.00
ATOM	1144	CG	ASP	Α	947	61.242	46.473	26.549	1.00 20.00
ATOM	1145	OD1	ASP	A	947	61.770	45.561	27.247	1.00 20.00
MOTA	1146	OD2	ASP	Α	947	60.447	46.255	25.595	1.00 20.00
MOTA	1148	N	VAL	Α	948	62.640	50.465	27.811	1.00 20.00
MOTA	1149	CA	VAL	Α	948	63.203	51.808	27.624	1.00 20.00
MOTA	1150	C	VAL	Α	948	64.337	52.099	28.598	1.00 20.00
ATOM	1151	0	VAL	Α	948	65.360	52.539	28.177	1.00 20.00
MOTA	1152	CB	VAL	Α	948	62.108	52.917	27.776	1.00 20.00
MOTA	1153	CG1	VAL	A	948	62.712	54.286	27.666	1.00 20.00
ATOM	1154	CG2	VAL	Α	948	61.121	52.784	26.722	1.00 20.00
ATOM	1156	N	ALA	Α	949	64.166	51.850	29.886	1.00 20.00
ATOM	1157	CA	ALA	Α	949	65.243	52.135	30.812	1.00 20.00
ATOM	1158	C	ALA			66.449	51.321	30.460	1.00 20.00
ATOM	1159	0	ALA			67.578	51.738	30.669	1.00 20.00
ATOM	1160	CB	ALA			64.850	51.822	32.209	1.00 20.00
ATOM	1162	M	ARG			66.212	50.134	29.928	1.00 20.00
MOTA	1163	CA	ARG			67.293	49.254	29.578	1.00 20.00
ATOM	1164	C	ARG			68.005	49.853	28.406	1.00 20.00
ATOM	1165	0	ARG			69.110	50.330	28.534	1.00 20.00
MOTA	1166	CB	ARG			66.762	47.872	29.240	1.00 20.00
MOTA	1167	CG	ARG			67.029	46.827	30.351	1.00 20.00
ATOM	1168	CD	ARG			67.033	45.384	29.809	1.00 20.00
ATOM	1169	NE	ARG			65.891	45.157	28.900	1.00 20.00
ATOM	1170	CZ	ARG			64.646	44.807	29.260	1.00 20.00
MOTA	1171	NH1	ARG			64.301	44.610	30.522	1.00 20.00
MOTA	1172	NH2	ARG			63.726	44.693	28.323	1.00 20.00
MOTA	1179	Ñ	GLY			67.390	49.844	27.248	1.00 20.00
ATOM	1180	CA	GLY			68.105	50.427	26.146	1.00 20.00
ATOM	1181	C	GLY		951	68.769	51.722	26.564	1.00 20.00
ATOM	1182	0	GLY			69.885	52.024	26.163	1.00 20.00
ATOM	1184	N			952	68.080	52.500	27.386	1.00 20.00
ATOM	1185	CA	MET			68.605	53.787	27.807	1.00 20.00
ATOM ATOM	1186 1187	C			952	69.952	53.633	28.437	1.00 20.00
ATOM	1188	CB	MET		952	70.949	53.969	27.845	1.00 20.00
ATON	1108	CD	ME I	М	222	67.659	54.492	28.797	1.00 20.00

ATOM	1189	CG	MET	Δ	952	67.289	55.894	28.400	1.00 20.00
MOTA	1190	SD	MET			67.360	56.078	26.632	1.00 20.00
ATOM	1191	CE	MET			68.656	57.374	26.554	1.00 20.00
ATOM	1193	N	ASP			69.903	53.096	29.648	1.00 20.00
ATOM	1194	CA	ASP			70.999	52.819	30.539	1.00 20.00
ATOM	1195	C	ASP			72,126	52.077	29.948	1.00 20.00
ATOM	1196	ō	ASP			73.077	51.814	30.608	1.00 20.00
ATOM	1197	CB	ASP			70.496	52.036	31,733	1.00 20.00
ATOM	1198	CG	ASP		953	71,538	51.117	32.295	1.00 20.00
ATOM	1199	OD1	ASP			72.241	51.480	33.245	1.00 20.00
ATOM	1200	OD2	ASP			71.672	50.004	31.785	1.00 20.00
ATOM	1202	N	TYR			72.025	51.743	28.692	1.00 20.00
ATOM	1203	CA	TYR		954	73.060	51.020	28.034	1.00 20.00
ATOM	1204	C	TYR			73.930	52.011	27.324	1.00 20.00
ATOM	1205	ō	TYR			75.135	51.833	27.254	1.00 20.00
ATOM	1206	CB	TYR			72.416	50.047	27.070	1.00 20.00
ATOM	1207	CG	TYR			73.330	49.432	26.068	1.00 20.00
ATOM	1208	CD1	TYR			74.294	48.485	26.442	1.00 20.00
ATOM	1209	CD2	TYR			73.181	49.719	24.734	1.00 20.00
ATOM	1210	CE1	TYR			75.071	47.839	25.483	1.00 20.00
ATOM	1211	CE2	TYR			73.947	49.082	23.779	1.00 20.00
ATOM	1212	CZ	TYR			74.883	48.136	24.153	1.00 20.00
ATOM	1213	OH	TYR			75.525	47.442	23.152	1.00 20.00
ATOM	1216	N	LEU			73.286	53.052	26.786	1.00 20.00
ATOM	1217	CA	LEU			73.908	54.184	26.069	1.00 20.00
ATOM	1218	C	LEU			74.356	55.110	27.176	1.00 20.00
ATOM	1219	ō	LEU		955	75.441	55.609	27.207	1.00 20.00
ATOM	1220	CB	LEU		955	72.863	54.943	25.265	1.00 20.00
ATOM	1221	CG	LEU			72.005	54.277	24.181	1.00 20.00
ATOM	1222	CD1	LEU			70.489	54.637	24.288	1.00 20.00
ATOM	1223	CD2	LEU			72.573	54.751	22.838	1.00 20.00
MOTA	1225	N	SER			73.465	55.311	28.113	1.00 20.00
ATOM	1226	CA	SER			73.699	56.176	29.209	1.00 20.00
ATOM	1227	С	SER			74.985	55.783	29.829	1.00 20.00
ATOM	1228	ō	SER			75.557	56.555	30.600	1.00 20.00
ATOM	1229	CB	SER			72.534	56.068	30.172	1.00 20.00
ATOM	1230	OG	SER			72.960	56.102	31.513	1.00 20.00
ATOM	1233	N	GLN			75.468	54.594	29.495	1.00 20.00
ATOM	1234	CA	GLN			76.755	54.097	30.040	1.00 20.00
ATOM	1235	С	GLN			77.824	54.054	28.959	1.00 20.00
MOTA	1236	0	GLN			78.985	54.213	29.208	1.00 20.00
ATOM	1237	CB	GLN	А	957	76.591	52.703	30.617	1.00 20.00
ATOM	1238	CG	GLN	Α	957	75.563	52.626	31.692	1.00 20.00
ATOM	1239	CD	GLN		957	76.088	51.882	32.875	1.00 20.00
ATOM	1240	OE1	GLN			77.083	52.314	33.492	1.00 20.00
ATOM	1241	NE2	GLN			75.447	50.747	33.215	1.00 20.00
MOTA	1245	N	LYS		958	77.396	53.827	27.747	1.00 20.00
ATOM	1246	CA	LYS			78.273	53.813	26.622	1.00 20.00
ATOM	1247	C			958	78.801	55.275	26.542	1.00 20.00
ATOM	1248	ō	LYS			79.643	55.627	25.704	1.00 20.00
ATOM	1249	CB			958	77.427	53.440	25.379	1.00 20.00
ATOM	1250	CG	LYS			78.110	52.552	24.355	1.00 20.00
ATOM	1251	CD	LYS			78.715	51.303	25.011	1.00 20.00
ATOM	1252	CE	LYS		958	77.845	50.099	24.743	1.00 20.00
ATOM	1253	NZ	LYS			77.570	50.041	23.271	1.00 20.00
ATOM	1258	N	GLN		959	78.268	56.108	27.436	1.00 20.00
ATOM	1259	CA	GLN			78.526	57.551	27.543	1.00 20.00
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Docket/App No.: 2079.1037-001 Title: Method of Identifying Inhibitors of TIE-2

Inventors: Nancy J. Bump etal.

ATOM	1260	С	GLA	Γ Δ	959	77.366	58.361	26.838	1.00 20.00
ATOM	1261	o	GLN		959	76.848	59.327	27.401	1.00 20.00
ATOM	1262	CB	GLN		959	79.901	57.893	26.973	1.00 20.00
ATOM	1263	CG	GLN		959	80.490	59.183	27.492	1.00 20.00
ATOM	1264	CD	GLN		959	80.934	59.114	28.944	1.00 20.00
ATOM	1265	OE1			959	81.840	58.313	29.295	1.00 20.00
ATOM	1266	NE2			959	80.332	59.979	29.811	1.00 20.00
ATOM	1270	N	PHE		960	76.937	57.940	25.649	1.00 20.00
ATOM	1271	CA	PHE		960	75.828	58.582	24.898	1.00 20.00
ATOM	1272	C			960	74.667	59.365	25.618	1.00 20.00
ATOM	1273	0	PHE		960	74.110	58.916	26.628	1.00 20.00
ATOM	1274	CB	PHE		960	75.189	57.528	23.985	1.00 20.00
ATOM	1275	CG	PHE		960	76.070	57.067	22.851	1.00 20.00
ATOM	1276	CD1	PHE		960	76.570	55.766	22.818	1.00 20.00
ATOM	1277	CD2	PHE		960	76.367	57.901	21.792	1.00 20.00
ATOM	1278	CE1	PHE		960	77.349	55.308	21.743	1.00 20.00
ATOM	1279	CE2	PHE	Α	960	77.148	57.442	20.720	1.00 20.00
ATOM	1280	CZ			960	77.636	56.142	20.720	1.00 20.00
ATOM	1282	N			961	74.308	60.532	25.068	1.00 20.00
ATOM	1283	CA	ILE		961	73.212	61.377	25.623	1.00 20.00
ATOM	1284	C			961	72.076	61.460	24.611	1.00 20.00
ATOM	1285	0	ILE		961	72.341	61.698	23.434	1.00 20.00
ATOM	1286	CB			961	73.631	62.832	25.918	1.00 20.00
ATOM	1287	CG1	ILE		961	74.862	62.886	26.840	1.00 20.00
ATOM	1288	CG2	ILE			72.489	63.547	26.600	1.00 20.00
ATOM	1289	CD1	ILE			75.935	63.855	26.373	1.00 20.00
ATOM	1291	N	HIS	А	962	70.821	61.314	25.049	1.00 20.00
ATOM	1292	CA	HIS		962	69.704	61.307	24.088	1.00 20.00
MOTA	1293	C	HIS	Α	962	69.158	62.604	23.535	1.00 20.00
ATOM	1294	0	HIS	Α	962	69.296	62.872	22.344	1.00 20.00
ATOM	1295	CB	HIS	Α	962	68.515	60.516	24.641	1.00 20.00
MOTA	1296	CG	HIS	Α	962	67.658	59.896	23.580	1.00 20.00
ATOM	1297	ND1	HIS	Α	962	67.259	58.586	23.621	1.00 20.00
ATOM	1298	CD2	HIS	Α	962	67.192	60.388	22.416	1.00 20.00
ATOM	1299	CE1	HIS	Α	962	66.589	58.290	22.528	1.00 20.00
ATOM	1300	NE2	HIS	Α	962	66.538	59.369	21.780	1.00 20.00
ATOM	1304	N	ARG	Α	963	68.502	63.363	24.413	1.00 20.00
MOTA	1305	CA	ARG	Α	963	67.848	64.665	24.122	1.00 20.00
ATOM	1306	C	ARG	A	963	66.653	64.636	23.125	1.00 20.00
ATOM	1307	0	ARG	Α	963	66.561	65.380	22.147	1.00 20.00
MOTA	1308	CB	ARG			68.909	65.724	23.726	1.00 20.00
MOTA	1309	CG	ARG			69.366	65.645	22.334	1.00 20.00
ATOM	1310	CD	ARG			70.710	66.180	22.216	1.00 20.00
ATOM	1311	NE	ARG	А	963	71.391	65.521	21.127	1.00 20.00
ATOM	1312	CZ	ARG			71.002	65.603	19.873	1.00 20.00
ATOM	1313	NH1	ARG	А	963	69.946	66.323	19.584	1.00 20.00
ATOM	1314	NH2	ARG	Α	963	71.648	64.941	18.925	1.00 20.00
ATOM	1321	N	ASN		964	65.705	63.767	23.408	1.00 20.00
ATOM	1322	CA	ASN	Α	964	64.536	63.623	22.545	1.00 20.00
ATOM	1323	C			964	63.904	62.262	22.803	1.00 20.00
ATOM	1324	0	ASN		964	63.497	61.558	21.890	1.00 20.00
ATOM	1325	CB	ASN			64.890	63.763	21.054	1.00 20.00
ATOM	1326	CG	ASN			63.647	63.940	20.206	1.00 20.00
ATOM	1327		ASN			62.565	64.079	20.780	1.00 20.00
ATOM	1328		ASN		964	63.769	63.939	18.866	1.00 20.00
ATOM	1332	N	LEU			63.861	61.914	24.081	1.00 20.00
ATOM	1333	CA	LEU	Α	965	63.291	60.665	24.546	1.00 20.00

ATOM	1334	С	LEU A	965	61.884	61.116	24.926	1.00	20.00
ATOM	1335	0	LEU A	965	61.701	62.119	25.629		20.00
ATOM	1336	CB	LEU A	965	64.079	60.172	25.769		20.00
ATOM	1337	CG	LEU A	965	64.292	58.716	26.189		20.00
ATOM	1338		LEU 2		64.689	57.802	25.040		20.00
ATOM	1339	CD2			65.320	58.728	27.27€		
ATOM	1341	N	ALA A		60.905				20.00
ATOM	1342	CA	ALA A		59.511	60.381	24.412		20.00
ATOM	1343	C	ALA A			60.666	24.605		20.00
ATOM	1344	0	ALA A		58.812	59.674	23.677		20.00
ATOM		CB			59.379	59.250	22.667		20.00
	1345		ALA A		59.244	62.056	24.189		20.00
MOTA	1347	N	ALA A		57.581	59.320	24.014	1.00	20.00
ATOM	1348	CA	ALA A		56.826	58.358	23.242	1.00	20.00
ATOM	1349	C	ALA A		56.842	58.489	21.740	1.00	20.00
ATOM	1350	0	ALA A		57.050	57.521	21.044	1.00	20.00
ATOM	1351	CB	ALA A		55.375	58.306	23.721	1.00	20.00
ATOM	1353	N	ARG A	968	56.606	59.671	21.205		20.00
ATOM	1354	CA	ARG A	968	56.580	59.697	19.759		20.00
ATOM	1355	C	ARG A	968	57.802	59.015	19.160		20.00
ATOM	1356	0	ARG A	968	57.751	58.532	18.041		20.00
ATOM	1357	CB	ARG A	968	56.455	61.123	19.226		20.00
ATOM	1358	CG	ARG A		57.264	62.162	19.987		20.00
ATOM	1359	CD	ARG A		57.684	63.354	19.087		
ATOM	1360	NE	ARG A		58.467				20.00
ATOM	1361	CZ	ARG A			64.376	19.784		20.00
ATOM	1362	NH1	ARG A		58.098	64.982	20.904		20.00
ATOM	1363	NH2	ARG A		56.937	64.698	21.492		20.00
ATOM	1370	N IN			58.929	65.828	21.473		20.00
ATOM	1371	CA	ASN A		58.881	58.913	19.931		20.00
ATOM	1371		ASN A		60.122	58.388	19.383		20.00
		C	ASN A		60.608	57.008	19.754		20.00
ATOM	1373	0	ASN A		61.716	56.647	19.413	1.00	20.00
ATOM	1374	CB	ASN A		61.232	59.407	19.630	1.00	20.00
ATOM	1375	CG	ASN A		60.873	60.787	19.118	1.00	20.00
MOTA	1376	OD1	ASN A		60.733	61.724	19.892	1.00	20.00
ATOM	1377	ND2	ASN A		60.702	60.910	17.802	1.00	20.00
ATOM	1381	N	ILE A	970	59.775	56.249	20.443	1.00	
ATOM	1382	CA	ILE A	970	60.073	54.912	20.851		20.00
ATOM	1383	C	ILE A	970	59.153	54.057	20.034		20.00
ATOM	1384	0	ILE A	970	58.006	54.384	19.930		20.00
ATOM	1385	CB	ILE A	970	59.717	54.770	22.294	1.00	
ATOM	1386	CG1	ILE A	970	60.699	55.565	23.110	1.00	
ATOM	1387	CG2	ILE A	970	59.730	53.328	22.724	1.00	
ATOM	1388	CD1	ILE A	970	60.800	55.095	24.515	1.00	
ATOM	1390	N	LEU A		59.626	52.971	19.435	1.00	
ATOM	1391	CA		971	58.733	52.086			
ATOM	1392	C	LEU A	971	58.290		18.656	1.00	
ATOM	1393	ō	LEU A	971		50.891	19.444	1.00	
ATOM	1394	CB			58.776	50.653	20.523	1.00	
ATOM	1395	CG		971	59.422	51.582	17.418	1.00	
ATOM			LEU A	971	59.930	52.837	16.785	1.00	
	1396		LEU A	971	61.161	52.652	16.019	1.00	
ATOM	1397		LEU A	971	58.844	53.290	15.909	1.00	20.00
ATOM	1399	N	VAL A	972	57.305	50.171	18.929	1.00	20.00
ATOM	1400	CA	A LAV	972	56.894	48.941	19.594	1.00	20.00
ATOM	1401	С		972	57.044	47.883	18.541	1.00	
ATOM	1402	0		972	56.221	47.793	17.661		20.00
ATOM	1403	CB	VAL A	972	55.492	48.932	20.043	1.00	
ATOM	1404	CGl	VAL A	972	55.224	47.588	20.632	1.00	

ATOM	1405	CG2	VAL A	9	72	55.264	50.012	21.107	1.00	20.00
ATOM	1407	N	GLY A		73	58.127	47.106	18.614	1.00	
ATOM	1408	CA	GLY A		73	58.375	46.109	17.614	1.00	20.00
ATOM	1409	C	GLY A		73	58.065	44.685	17.980	1.00	
			GLY A		73	57.370		18.927	1.00	
ATOM	1410	0					44.393			
MOTA	1412	N	GLU A		74	58.€12	43.793	17.178		20.00
ATOM	1413	CA	GLU A		74	58.445	42.383	17.357	1.00	
MOTA	1414	С	GLU A		74	58.379	41.981	18.795		20.00
ATOM	1415	0	GLU A		74	59.246	42.274	19.572	1.00	20.00
ATOM	1416	CB	GLU A		74	59.568	41.648	16.671	1.00	20.00
MOTA	1417	CG	GLU A		74	59.187	41.010	15.343	1.00	20.00
ATOM	1418	CD	GLU A	. 9	74	57.698	41.173	14.936	1.00	20.00
MOTA	1419	OEl	GLU A	. 9	74	56.763	40.870	15.733	1.00	20.00
ATOM	1420	OE2	GLU A	. 9	74	57.467	41.592	13.780	1.00	20.00
ATOM	1422	N	ASN A	. 9	75	57.305	41.316	19.147	1.00	20.00
ATOM	1423	CA	ASN A	. 9	75	57.119	40.830	20.483	1.00	20.00
ATOM	1424	C	ASN A	. 9	75	56.741	41.832	21.554	1.00	20.00
ATOM	1425	0	ASN A		75	56.811	41.544	22.758		20.00
ATOM	1426	CB	ASN A		75	58.333	40.006	20.864		20.00
ATOM	1427	CG	ASN A		75	58.189	38.519	20.428		20.00
ATOM	1428		ASN A		75	58.243	37.639	21.263		20.00
ATOM	1429	ND2	ASN A			57.988	38.266	19.136	1.00	
ATOM	1433	N	TYR A			56.299		21.103		20.00
							43.003			
ATOM	1434	CA	TYR A			55.839	44.047	21.988	1.00	
ATOM	1435	C	TYR A			56.946	44.589	22.839		20.00
ATOM	1436	0	TYR A			56.797	44.863	24.016	1.00	
ATOM	1437	CB	TYR A			54.684	43.498	22.830		20.00
ATOM	1438	CG	TYR A			53.466	43.191	21.993		20.00
ATOM	1439		TYR A			52.878	41.927	22.017		20.00
ATOM	1440	CD2	TYR A			52.939	44.157	21.112		20.00
ATOM	1441	CE1				51.801	41.624	21.182		20.00
MOTA	1442	CE2	TYR A	. 9	76	51.874	43.870	20.279	1.00	20.00
ATOM	1443	CZ	TYR A	9	76	51.306	42.604	20.307	1.00	20.00
ATOM	1444	OH	TYR A	. 9	76	50.273	42.291	19.427	1.00	20.00
ATOM	1447	N	VAL 3	9	77	58.070	44.787	22.191	1.00	20.00
ATOM	1448	CA	VAL A	9	77	59.260	45.295	22.845	1.00	20.00
ATOM	1449	C	VAL A	9	77	59.536	46.766	22.497	1.00	20.00
ATOM	1450	0	VAL A	. 9	77	59.446	47.195	21.355	1.00	20.00
ATOM	1451	CB	VAL 1	. 9	977	60.514	44.377	22.485	1.00	20.00
ATOM	1452	CG1				61.768	44.854	23.182	1.00	
ATOM	1453		VAL A			60.230	42.943	22.890	1.00	20.00
ATOM	1455	N	ALA A			59.839	47.529	23.525	1.00	
ATOM	1456	CA	ALA A			60.174	48.898	23.328	1.00	
ATOM	1457	C	ALA A			61.434	48.921	22.476	1.00	20.00
ATOM	1458	0	ALA A			62.242	48.026	22.470	1.00	
ATOM									1.00	20.00
	1459	CB	ALA A			60.423	49.546	24.643		20.00
ATOM	1461	N	LYS A			61.597	49.926	21.653		
ATOM	1462	CA	LYS A			62.791	50.005	20.864	1.00	
ATOM	1463	С	LYS 2			63.098	51.476	20.826		20.00
ATOM	1464	0	LYS I			62.263	52.262	20.387		20.00
ATOM	1465	CB	LYS A			62.551	49.492	19.448	1.00	
ATOM	1466	CG	LYS 2			62.076	48.043	19.369		20.00
ATOM	1467	CD	LYS /		979	63.115	47.009	19.864	1.00	20.00
ATOM	1468	CE	LYS 2	. 9	979	63.866	46.343	18.708	1.00	20.00
ATOM	1469	NZ	LYS 3	4 9	979	63.212	45.122	18.253	1.00	20.00
ATOM	1474	N	ILE A	4 9	980	64.274	51.873	21.302	1.00	20.00
ATOM	1475	CA	ILE 2	1 9	980	64.615	53.287	21.240	1.00	20.00

ATOM	1476	С	TLE	70	980	65.131	53.691	19.858	3 00	20.00
ATOM	1477	o			980	65.938	53.004	19.838	1.00	20.00
ATOM	1478	СВ			980	65.671				
ATOM	1479	CG1	ILE			65.205	53.665	22.263		20.00
ATOM	1480	CG2	ILE				53.311	23.667	1.00	20.00
ATOM						65.943	55.135	22.173		20.00
	1481	CD1	ILE			66.262	53.521	24.730	1.00	20.00
ATOM	1483	N	ALA			64.629	54.815	19.383		20.00
ATOM	1484	CA	ALA		981	65.038	55.342	18.097		20.00
ATOM	1485	C	ALA		981	65.244	56.854	18.141		20.00
ATOM	1486	0	ALA			65.039	57.530	19.172	1.00	20.00
ATOM	1487	CB	ALA			64.024	55.024	17.060		20.00
ATOM	1489	N	ASP		982	65.610	57.362	16.973		20.00
ATOM	1490	CA	ASP		982	65.888	58.763	16.721	1.00	20.00
ATOM	1491	C	ASP		982	66.653	59.517	17.801	1.00	20.00
ATOM	1492	0			982	66.041	60.135	18.684	1.00	20.00
MOTA	1493	CB	ASP	A	982	64.620	59.527	16.416	1.00	20.00
ATOM	1494	CG	ASP		982	64.911	60.946	16.122	1.00	20.00
ATOM	1495	OD1	ASP	Α	982	65.455	61.240	15.031	1.00	20.00
ATOM	1496	OD2	ASP	Α	982	64.626	61.766	16.998	1.00	20.00
ATOM	1498	N	PHE	Α	983	67.988	59.525	17.706	1.00	20.00
ATOM	1499	CA	PHE	Α	983	68.770	60.223	18.733		20.00
ATOM	1500	С	PHE	Α	983	70.123	60.755	18.312	1.00	20.00
ATOM	1501	0	PHE	Α	983	70.565	60.712	17.155		20.00
ATOM	1502	CB	PHE	А	983	69.001	59.327	19.948		20.00
ATOM	1503	CG	PHE	А	983	69.411	57.928	19.589		20.00
ATOM	1504	CD1	PHE	А	983	68.856	57.280	18.452		20.00
ATOM	1505	CD2				70.310	57.244	20.375		20.00
ATOM	1506	CE1			983	69.181	55.987	18.106		20.00
MOTA	1507	CE2	PHE			70.648	55.939	20.044	1.00	
ATOM	1508	CZ			983	70.075	55.308	18.895		20.00
MOTA	1510	N	GLY			70.797	61.274	19.305		20.00
ATOM	1511	CA			984	72.082	61.799	19.010	1.00	20.00
ATOM	1512	C	GLY			73.058	60.661	18.913	1.00	20.00
MOTA	1513	ō	GLY			72.980	59.633	19.633		20.00
ATOM	1515	N	LEU			73.978	60.846	17.977	1.00	20.00
ATOM	1516	CA	LEU		985	75.055	59.913	17.812	1.00	
ATOM	1517	C	LEU		985	76.044	60.741	18.669	1.00	20.00
ATOM	1518	ō	LEU			77.236	60.872	18.323	1.00	20.00
ATOM	1519	CB			985	75.483	59.871	16.342	1.00	20.00
ATOM	1520	CG	LEU		985	75.093				
ATOM	1521	CD1	LEU		985	75.645	58.770 57.463	15.337 15.830	1.00	20.00
ATOM	1522	CD2	LEU			73.545				
ATOM	1524	N N	SER			75.561	58.659	15.129	1.00	20.00
ATOM	1525	CA	SER			76.443	61.306	19.786	1.00	20.00
ATOM	1526	C	SER			76.443	62.118	20.611	1.00	20.00
ATOM	1527	0	SER				61.629	21.970	1.00	20.00
ATOM	1528	CB	SER		986	76.169	61.709	22.937	1.00	20.00
ATOM	1529	OG	SER			75.850	63.504	20.815	1.00	20.00
ATOM.	1532					76.764	64.504	20.379	1.00	20.00
ATOM	1532	N	ARG		987	78.189	61.152	22.037	1.00	20.00
		CA	ARG		987	78.763	60.709	23.306	1.00	20.00
ATOM	1534	С	ARG		987	79.511	61.893	23.794	1.00	20.00
ATOM	1535	0	ARG		987	80.191	62.578	23.059	1.00	20.00
ATOM	1536	CB	ARG		987	79.752	59.525	23.214	1.00	20.00
ATOM	1537	CG	ARG		987	79.583	58.534	22.078	1.00	20.00
ATOM	1538	CD	ARG		987	80.953	58.120	21.459	1.00	20.00
MOTA	1539	NE	ARG		987	81.908	57.509	22.396	1.00	20.00
ATOM	1540	CZ	ARG	A	987	82.932	56.731	22.021	1.00	20.00

 $\begin{array}{ll} \mbox{Docket/App No.:} & 2079.1037-001 \\ \mbox{Title: Method of Identifying Inhibitors of TIE-2} \\ \mbox{Inventors:} & \mbox{Nancy J. Bump $\it{et al}$.} \end{array}$

ATOM	1541	NH1	ARG	Α	987	83.127	56.473	20.738	1.00 20.00
MOTA	1542	NH2	ARG	A	987	83.761	56.206	22.936	1.00 20.00
ATOM	1549	N	GLY	A	988	79.387	62.122	25.068	1.00 20.00
ATOM	1550	CA	GLY	A	988	80.028	63.260	25.633	1.00 20.00
MOTA	1551	C	GLY	Α	988	79.480	63.223	27.024	1.00 20.00
ATOM	1552	0	GLY	A	988	79.050	62.151	27.453	1.00 20.00
ATOM	1554	N	GLN	A	989	79.521	64.369	27.704	1.00 20.00
ATOM	1555	CA	GLN	Α	989	79.020	64.579	29.053	1.00 20.00
ATOM	1556	C	GLN	Α	989	78.115	65.864	29.062	1.00 20.00
MOTA	1557	0	GLN	Α	989	77.565	66.257	30.075	1.00 20.00
MOTA	1558	CB	GLN	A	989	80.219	64.739	29.974	1.00 20.00
ATOM	1559	CG	GLN	A	989	79.924	65.292	31.348	1.00 20.00
MOTA	1560	CD	GLN	Α	989	81.068	66.095	31.985	1.00 20.00
MOTA	1561	OE1	GLN			81.783	66.897	31.332	1.00 20.00
MOTA	1562	NE2	GLN	Α	989	81.233	65.891	33.273	1.00 20.00
ATOM	1566	N	GLU	Α	990	77.933	66.496	27.908	1.00 20.00
ATOM	1567	CA	GLU		990	77.185	67.704	27.889	1.00 20.00
ATOM	1568	С	GLU	A	990	76.348	68.030	26.675	1.00 20.00
ATOM	1569	0	GLU		990	75.199	68.420	26.836	1.00 20.00
ATOM	1570	CB	GLU			78.134	68.853	28.117	1.00 20.00
ATOM	1571	CG	GLU			78.194	69.367	29.499	1.00 20.00
ATOM	1572	CD	GLU			79.467	68.991	30.151	1.00 20.00
ATOM	1573	OE1	GLU			80.437	68.623	29.443	1.00 20.00
ATOM	1574	OE2	GLU			79.486	69.061	31.387	1.00 20.00
ATOM	1576	N	VAL			76.878	67.895	25.469	1.00 20.00
ATOM	1577	CA	VAL			76.098	68.270	24.274	1.00 20.00
ATOM	1578	c	VAL			75.373	69.616	24.400	1.00 20.00
ATOM	1579	ō	VAL			74.538	69.823	25.274	1.00 20.00
ATOM	1580	CB	VAL		991	74.965	67.324	23.910	1.00 20.00
ATOM	1581	CGl	VAL			74.620	67.527	22.479	1.00 20.00
ATOM	1582	CG2	VAL			75.323	65.922	24.159	1.00 20.00
ATOM	1584	N	TYR			75.674	70.528	23.504	1.00 20.00
ATOM	1585	CA	TYR		992	74.997	71.780	23.514	1.00 20.00
ATOM	1586	C	TYR			74.389	71.784	22.118	1.00 20.00
ATOM	1587	ō	TYR			75.036	71.437	21.138	1.00 20.00
ATOM	1588	CB	TYR			76.003	72.945	23.687	1.00 20.00
ATOM	1589	CG	TYR	А	992	75.520	74.227	23.027	1.00 20.00
ATOM	1590	CD1	TYR			74.579	75.023	23.654	1.00 20.00
ATOM	1591	CD2	TYR	Α	992	75.804	74.487	21.702	1.00 20.00
ATOM	1592	CE1	TYR			73.939	75.989	22.987	1.00 20.00
ATOM	1593	CE2	TYR			75.160	75.453	21.044	1.00 20.00
ATOM	1594	CZ	TYR			74.218	76.200	21.690	1.00 20.00
ATOM	1595	OH	TYR			73.552	77.196	21.023	1.00 20.00
ATOM	1598	N	VAL			73.131	72.161	22.020	1.00 20.00
ATOM	1599	CA	VAL		993	72.482	72.226	20.712	1.00 20.00
ATOM	1600	C	VAL			71.311	73.168	21.008	1.00 20.00
ATOM	1601	0	VAL			70.748	73.116	22.101	1.00 20.00
ATOM	1602	CB	VAL			72.102	70.746	20.159	1.00 20.00
ATOM	1603	CG1	VAL		993	71.570	69.843	21.226	1.00 20.00
ATOM	1604	CG2	VAL			71.121	70.843	19.076	1.00 20.00
MOTA	1606	N	LYS		994	70.990	74.076	20.082	1.00 20.00
ATOM	1607	CA	LYS		994	69.917	75.099	20.335	1.00 20.00
ATOM	1608	C	LYS		994	69.171	75.616	19.093	1.00 20.00
ATOM	1609	0		Ā	994	69.784	76.097	18.105	1.00 20.00
ATOM	1610	CB		A	994	70.508	76.336	21.083	1.00 20.00
ATOM	1611	CG	LYS		994	69.513	77.422	21.498	1.00 20.00
ATOM	1612	CD	LYS		994	69.827	78.812	20.847	1.00 20.00
	2022		220	**		00.027	.0.012	20.047	

ATOM 1613 CE LYS A 994
ATOM 1614 NZ LYS A 995
ATOM 1619 N LYS A 995
ATOM 1620 CA LYS A 995
ATOM 1621 C LYS A 995
ATOM 1622 C LYS A 995
ATOM 1622 C LYS A 995
ATOM 1623 CB LYS A 995
ATOM 1624 C LYS A 995
ATOM 1625 C LYS A 995
ATOM 1626 C LYS A 995
ATOM 1627
ATOM 1628 C LYS A 995
ATOM 1628 C LYS A 995
ATOM 1628 C LYS A 995
ATOM 1629 C LYS A 995
ATOM 1629 C LYS A 995
ATOM 1620 C LYS A 995
ATOM 1630 C LYS A 995
ATOM 1640 C LYS A 995
ATOM 164

ATOM	1687	С	ALA A	0.06	65.147	71.295	31.859	1.00 20.00
MCTA	1688	0	ALA A		65.854	71.804	30.965	1.00 20.00
ATOM	1689	CB	ALA A		65.819	68.944	32.215	1.00 20.00
ATOM	1691	N		007	64.694	71.961	32.930	1.00 20.00
ATOM	1692	CA		007	64.982	73.368	33.167	1.00 20.00
ATOM	1693	C		007	66.361	73.633	32.607	1.00 20.00
MOTA	1694	0		. 007		74.388		
ATOM	1695	CB		. 007	66.500		31.663	1.00 20.00
					64.876	73.725	34.674	1.00 20.00
ATOM	1696	CG1		. 007	65.897	72.943	35.501	1.00 20.00
ATOM	1697	CG2	ILE A		63.518	73.339	35.193	1.00 20.00
MOTA	1698	CD1		007	66.781	73.773	36.516	1.00 20.00
ATOM	1700	N	GLU A		67.361	72.921	33.131	1.00 20.00
ATOM	1701	CA	GLU A		68.768	73.052	32.719	1.00 20.00
ATOM	1702	C	GLU A		68.886	73.301	31.217	1.00 20.00
ATOM	1703	0	GLU A		69.401	74.319	30.811	1.00 20.00
ATOM	1704	CB	GLU A		69.565	71.799	33.174	1.00 20.00
MOTA	1705	CG	GLU A		69.424	70.540	32.296	1.00 20.00
ATOM	1706	CD	GLU A	800	69.290	69.267	33.131	1.00 20.00
ATOM	1707	OE1	GLU A	800	69.605	69.369	34.325	1.00 20.00
ATOM	1708	OE2	GLU A	800	68.867	68.187	32.613	1.00 20.00
ATOM	1710	N	SER A	009	68.388	72.388	30.384	1.00 20.00
ATOM	1711	CA	SER A	009	68.456	72.641	28.947	1.00 20.00
ATOM	1712	C	SER A	009	67.387	73.630	28.440	1.00 20.00
ATOM	1713	0	SER A	009	67.491	74.109	27.327	1.00 20.00
ATOM	1714	CB	SER A	009	68.424	71.329	28.129	1.00 20.00
ATOM	1715	OG	SER A	009	67.325	70.511	28.426	1.00 20.00
ATOM	1718	N	LEU A		66.361	73.915	29.246	1.00 20.00
ATOM	1719	CA	LEU A		65.328	74.909	28.869	1.00 20.00
MOTA	1720	C	LEU A		66.043	76.294	28.797	1.00 20.00
ATOM	1721	ō	LEU A		65.881	77.047	27.816	1.00 20.00
ATOM	1722	CB	LEU A		64.213	74.966	29.928	1.00 20.00
ATOM	1723	CG	LEU A		62.880	74.229	29.760	1.00 20.00
ATOM	1724	CD1	LEU A		61.863	75.034	30.483	1.00 20.00
ATOM	1725		LEU A		62.459	74.066	28.330	1.00 20.00
ATOM	1727	N		011	66.825	76.577	29.854	1.00 20.00
ATOM	1728	CA	ASN A		67.663	77.762	30.020	1.00 20.00
ATOM	1729	C	ASN A		68.799	77.692	28.983	1.00 20.00
MOTA	1730	0		011	68.799	78.348	27.914	1.00 20.00
ATOM	1731	CB		011	68.303	77.725	31.386	1.00 20.00
ATOM	1732	CG	ASN A				32.474	1.00 20.00
ATOM	1733			011	67.325 66.150	77.469 77.759	32.474	1.00 20.00
ATOM	1734	ND2						
ATOM	1738		ASN A		67.791	76.929	33.607	1.00 20.00
ATOM		N		012	69.774	76.859	29.325	1.00 20.00
ATOM	1739 1740	CA C	TYR A		70.918	76.611	28.481	1.00 20.00
			TYR A		70.488	75.487	27.544	1.00 20.00
ATOM	1741	0	TYR A		69.908	74.499	28.020	1.00 20.00
MOTA	1742	CB	TYR A		72.047	76.179	29.370	1.00 20.00
ATOM	1743	CG	TYR A		71.787	76.590	30.784	1.00 20.00
ATOM	1744		TYR A		71.854	75.680	31.809	1.00 20.00
ATOM	1745	CD2	TYR A		71.474	77.879	31.097	1.00 20.00
ATOM	1746	CE1	TYR A		71.619	76.047	33.097	1.00 20.00
MOTA	1747	CE2	TYR A		71.246	78.242	32.357	1.00 20.00
MOTA	1748	CZ	TYR A	012	71.321	77.328	33.361	1.00 20.00
ATOM	1749	OH	TYR A	012	71.143	77.709	34.668	1.00 20.00
ATOM	1752	N	SER A	013	70.711	75.615	26.235	1.00 20.00
ATOM	1753	CA	SER A	013	70.309	74.544	25.335	1.00 20.00
ATOM	1754	C	SER A	013	71.274	73.385	25.467	1.00 20.00

ATOM	1755	0	SER	Δ	013	71.810	72.898	24.464	1.00 20.00
ATOM	1756	CB	SER			70.291	75.025	23.898	1.00 20.00
ATOM	1757	OG	SER			70.122	76.432	23.813	1.00 20.00
ATOM	1760	N	VAL			71.469	72.957	26.713	1.00 20.00
		CA	VAL			72.378	71.890	27.084	1.00 20.00
ATOM	1761		VAL			71.711	70.603	27.571	1.00 20.00
ATOM	1762	C							1.00 20.00
ATOM	1763	0	VAL			70.895	70.613	28.493	
ATOM	1764	CB	VAL			73.316	72.316	28.230	1.00 20.00
ATOM	1765	CG1	VAL			74.335	73.331	27.748	1.00 20.00
ATOM	1766	CG2	VAL			72.490	72.849	29.394	1.00 20.00
ATOM	1768	N	TYR			72.100	69.472	27.009	1.00 20.00
ATOM	1769	CA	TYR			71.502	68.235	27.446	1.00 20.00
ATOM	1770	C	TYR			72.543	67.266	28.029	1.00 20.00
MOTA	1771	0	TYR	Α	015	73.619	67.072	27.494	1.00 20.00
MOTA	1772	CB	TYR	A	015	70.783	67.599	26.252	1.00 20.00
ATOM	1773	CG	TYR	Α	015	69.875	68.533	25.477	1.00 20.00
ATOM	1774	CD1	TYR	Α	015	70.194	68.918	24.179	1.00 20.00
ATOM	1775	CD2	TYR	Α	015	68.665	68.975	26.022	1.00 20.00
ATOM	1776	CE1	TYR	A	015	69.334	69.718	23.416	1.00 20.00
ATOM	1777	CE2	TYR	Α	015	67.782	69.778	25.286	1.00 20.00
ATOM	1778	CZ	TYR	Α	015	68.116	70.150	23.968	1.00 20.00
ATOM	1779	OH	TYR	Α	015	67.249	70.935	23.209	1.00 20.00
ATOM	1782	N	THR	А	016	72.253	66.679	29.161	1.00 20.00
ATOM	1783	CA	THR	А	016	73.172	65.695	29.673	1.00 20.00
ATOM	1784	С	THR	Α	016	72.464	64.347	29.834	1.00 20.00
ATOM	1785	ō	THR			71.573	63.995	29.086	1.00 20.00
ATOM	1786	CB	THR	А	016	73.717	66.097	31.000	1.00 20.00
ATOM	1787	OG1	THR			72.692	66.000	31.993	1.00 20.00
ATOM	1788	CG2	THR			74.253	67.455	30.909	1.00 20.00
ATOM	1791	N	THR			72.891	63.584	30.818	1.00 20.00
ATOM	1792	CA	THR			72.235	62.339	31.031	1.00 20.00
ATOM	1793	С	THR			71.021	62.785	31.819	1.00 20.00
ATOM	1794	ō	THR			69.889	62.570	31.364	1.00 20.00
ATOM	1795	CB	THR			73.112	61.308	31.826	1.00 20.00
ATOM	1796	OG1	THR			73.546	60.286	30.931	1.00 20.00
ATOM	1797	CG2	THR			72.315	60.660	32.954	1.00 20.00
ATOM	1800	N	ASN			71.265	63.454	32.958	1.00 20.00
ATOM	1801	CA	ASN			70.189	63.934	33.825	1.00 20.00
ATOM	1802	C	ASN			69.025	64.568	33.108	1.00 20.00
ATOM	1803	0	ASN			67.937	64.530	33.636	1.00 20.00
ATOM	1804	CB	ASN			70.696	64.904	34.868	1.00 20.00
ATOM	1805	CG	ASN			71.785	64.331	35.676	1.00 20.00
ATOM	1806		ASN			71.761	64.412	36.887	1.00 20.00
ATOM	1807		ASN			72.767	63.734	35.013	1.00 20.00
ATOM	1811	N	SER			69.247	65.184	31.948	1.00 20.00
ATOM	1812	CA	SER			68.132	65.740	31.199	1.00 20.00
ATOM	1813	C	SER			67.362	64.513	30.704	1.00 20.00
ATOM	1814	0	SER			66.145	64.414	30.875	1.00 20.00
							66.544	30.006	1.00 20.00
ATOM	1815	CB	SER			68.613 69.999		30.051	1.00 20.00
ATOM	1816	OG	SER		020		66.633 63.583	30.051	1.00 20.00
ATOM	1819	N				68.110			1.00 20.00
ATOM	1820	CA				67.596	62.309	29.604	1.00 20.00
MOTA	1821	C	ASP			66.784	61.679	30.741	
ATOM	1822	0			020	65.672	61.194	30.543	
ATOM	1823	CB	ASP		020	68.767	61.388	29.217	1.00 20.00
ATOM	1824	CG			020	69.154	61.484	27.729	
ATOM	1825	OD1	ASP	Α	020	68.649	62.363	26.979	1.00 20.00

Title: Method o	of Identifying	Inhibitors of TIE-2
Inventors:		Bump et al.

ATOM	1826	002	ASP			69.992	60.673	27.292	1.00	20.00
ATOM	1828	N	VAL			67.294	61.728	31.955		20.00
ATOM	1829	CA	VAL			66.522	61.083	32.960		20.00
ATOM	1830	C	VAL	A	021	65.300	61.826	33.326	1.00	20.00
MOTA	1831	0	VAL			64.372	61.212	33.879		20.00
MOTA	1832	CB	VAL	A	C21	67.316	60.766	34.204	1.00	20.00
ATOM	1833	CG1	VAL	Α	021	66.471	60.862	35.417	1.00	20.00
ATOM	1834	CG2	VAL	A	021	67.803	59.362	34.110	1.00	20.00
MOTA	1836	N	TRP	Α	022	65.290	63.135	33.035	1.00	20.00
ATOM	1837	CA	TRP	Α	022	64.157	64.016	33.326	1.00	20.00
ATOM	1838	C	TRP	A	022	63.051	63.699	32.319	1.00	20.00
ATOM	1839	0	TRP	Α	022	61.948	63.268	32.629	1.00	20.00
ATOM	1840	CB	TRP	Α	022	64.596	65.468	33.160	1.00	20.00
ATOM	1841	CG	TRP	Α	022	63.439	66.467	33.254	1.00	20.00
ATOM	1842	CD1	TRP .	Α	022	62.437	66.648	32.337	1.00	20.00
ATOM	1843	CD2	TRP .	Α	022	63.161	67.366	34.322	1.00	20.00
ATOM	1844	NE1	TRP	Α	022	61.576	67.578	32.767	1.00	20.00
ATOM	1845	CE2	TRP	A	022	61.985	68.049	33.984	1.00	20.00
ATOM	1846	CE3	TRP .	A	022	63.791	67.662	35.529	1.00	20.00
ATOM	1847	CZ2	TRP .	Α	022	61.413	69.029	34.815	1.00	20.00
ATOM	1848	CZ3	TRP .	А	022	63.237	68.626	36.355	1.00	20.00
ATOM	1849	CH2	TRP	Α	022	62.052	69.303	35.992		20.00
ATOM	1852	N	SER .	Α	023	63.407	63.969	31.084		20.00
ATOM	1853	CA	SER .	А	023	62.591	63.721	29.928		20.00
ATOM	1854	C	SER .	A	023	61.978	62.316	30.007		20.00
ATOM	1855	0	SER .			60.863	62.092	29.540		20.00
ATOM	1856	CB	SER .			63.497	63.860	28.709		20.00
ATOM	1857	OG	SER .			62.747	63.795	27.527		20.00
ATOM	1860	N	TYR .	Α	024	62.731	61.390	30.617	1.00	20.00
ATOM	1861	CA	TYR .			62.361	59.980	30.801		20.00
ATOM	1862	C	TYR	Α	024	60.980	59.761	31.454		20.00
ATOM	1863	0	TYR .	A	024	60.137	58.991	30.967	1.00	20.00
ATOM	1864	CB	TYR .			63.436	59.307	31.627		20.00
ATOM	1865	CG	TYR .	А	024	63.129	57.866	31.859	1.00	20.00
ATOM	1866	CD1	TYR .	A	024	63.276	56.948	30.849		20.00
ATOM	1867	CD2	TYR .	А	024	62.479	57.473	33.019		20.00
ATOM	1868	CE1	TYR			62.766	55.706	30.979		20.00
ATOM	1869	CE2	TYR.			61.962	56.236	33.157		20.00
ATOM	1870	CZ	TYR .			62.099	55.365	32.135		20.00
ATOM	1871	ОН	TYR.	А	024	61.517	54.160	32.263		20.00
ATOM	1874	N	GLY .	Α	025	60.803	60.436	32.583		20.00
ATOM	1875	CA	GLY .	Α	025	59.558	60.427	33.311		20.00
ATOM	1876	С	GLY .			58.477	61.257	32.614		20.00
ATOM	1877	0	GLY .			57.365	61.290	33.058		20.00
ATOM	1879	N	VAL .			58.747	61.974	31.544		20.00
ATOM	1880	CA	VAL.			57.596	62.614	30.980		20.00
ATOM	1881	C	VAL .	A	026	57.057	61.313	30.484		20.00
ATOM	1882	ō	VAL .			56.006	60.906	30.923		20.00
ATOM	1883	CB	VAL .			57.889	63.625	29.823		20.00
ATOM	1884	CG1	VAL .			56.583	64.258	29.328		20.00
ATOM	1885	CG2	VAL .			58.746	64.717	30.327	1.00	
ATOM	1887	N	LEU .			57.843	60.639	29.632		20.00
ATOM	1888	CA	LEU .			57.535	59.273	29.064		20.00
ATOM	1889	C	LEU .		027	56.767	58.278	30.014		20.00
ATOM	1890	ō			027	55.745	57.736	29.702		20.00
ATOM	1891	CB	LEU			58.852	58.615	28.663		20.00
ATOM	1892	CG	LEU .			58.843	57.551	27.579		20.00

ATOM	1893	CDi	LEU	A	027	58.238	8 58.171	26.367	7 00	20.00
ATOM	1894	CD2				60.239		27.287	1.00	
ATOM	1896	N			028	57.333		31.171		20.00
ATOM	1897	CA			028	56.723		32.128	1.00	
ATOM	1898	C			028	55.330		32.128		20.00
ATOM	1899	0			028	54.428				
ATOM	1900	CB			028			32.517	1.00	
ATOM	1901	CG			028	57.455 56.778		33.427		20.00
ATOM	1902	CD1	LEU					34.430	1.00	
ATOM	1902	CD2	LEU			56.765		33.926		20.00
ATOM	1905	N N	TRP		028	57.488		35.740		20.00
ATOM						55.148		32.409		20.00
	1906	CA	TRP			53.820		32.612		20.00
ATOM	1907	C	TRP		029	53.028		31.295		20.00
ATOM	1908	0	TRP			51.869		31.301		20.00
MOTA	1909	CB	TRP			54.010		33.088		20.00
ATOM	1910	CG	TRP			52.746		33.293		20.00
ATOM	1911	CD1				52.207		34.483		20.00
ATOM	1912	CD2	TRP			51.934		32.271		20.00
ATOM	1913	NEl	TRP			51.113		34.241	1.00	20.00
ATOM	1914	CE2	TRP			50.925	63.138	32.892	1.00	20.00
ATOM	1915	CE3	TRP			51.962	62.298	30.886	1.00	20.00
ATOM	1916	CZ2	TRP			49.975	63.798	32.185	1.00	20.00
MOTA	1917	CZ3				51.018	62.951	30.186	1.00	20.00
ATOM	1918	CH2	TRP			50.030	63.701	30.830	1.00	20.00
ATOM	1921	N	GLU	Α	030	53.684	59.695	30.166	1.00	20.00
ATOM	1922	CA	GLU			53.067	59.537	28.861	1.00	20.00
MOTA	1923	C	GLU	А	030	52.592	58.103	28.823	1.00	20.00
ATOM	1924	0	GLU	A	030	51.775	57.758	27.982		20.00
ATOM	1925	CB	GLU	Α	030	54.099		27.737		20.00
ATOM	1926	CG	GLU	A	030	54.380		27.071		20.00
ATOM	1927	CD	GLU	A	030	55.162	60.706	25.771		20.00
ATOM	1928	OE1	GLU	Α	030	55.818	59.668	25.665		20.00
ATOM	1929	OE2	GLU	Α	030	55.144	61.535	24.838		20.00
ATOM	1931	N	ILE	А	031	53.124	57.260	29.711		20.00
ATOM	1932	CA	ILE	А	031	52.839	55.820	29.680		20.00
ATOM	1933	С	ILE			51.803	55.305	30.628	1.00	
ATOM	1934	0	ILE			50.931	54.585	30.219		20.00
ATOM	1935	CB	ILE			54.192	54.974	29.833		20.00
MOTA	1936	CG1	ILE			54.803	54.722	28.459		20.00
ATOM	1937	CG2	ILE			53.964	53.607	30.495		20.00
ATOM	1938	CD1	ILE			56.144	54.104	28.543		20.00
ATOM	1940	N	VAL			51.893	55.672	31.892		20.00
ATOM	1941	CA	VAL			50.918	55.223	32.895		20.00
ATOM	1942	C	VAL			49.618	55.914	32.620		20.00
ATOM	1943	ō	VAL			48.706	55.811	33.412		20.00
ATOM	1944	CB	VAL			51.306	55.664	34.327		20.00
ATOM	1945	CG1	VAL			50.610	56.932			
ATOM	1946	CG2	VAL					34.667		20.00
ATOM	1948	N N	SER			50.962	54.602	35.333		20.00
ATOM	1948	CA	SER			49.552	56.605	31.493		20.00
ATOM	1950	CA	SER			48.413	57.405	31.146		20.00
ATOM	1951					47.776	57.027	29.850	1.00	
ATOM		0	SER			46.634	57.396	29.585		20.00
	1952	CB	SER			48.828	58.889	31.116	1.00	20.00
ATOM	1953	OG	SER			49.492	59.239	29.905		20.00
ATOM	1956	N	LEU			48.513	56.329	29.019	1.00	
ATOM	1957	CA	LEU			47.975	55.904	27.758		20.00
ATOM	1958	С	LEU	Α	034	47.939	57.037	26.801	1.00	20.00

ATOM	1959	0	LEU A	034	46.917	57.357	26.219	1.00 20.00
ATOM	1960	CB	LEU A		46.580	55.366	27.923	1.00 20.00
ATOM	1961	CG	LEU A		46.208	54.020	28.500	1.00 20.00
ATOM	1962	CD1	LEU A		46.074	54.041	29.977	1.00 20.00
ATOM	1963	CD2	LEU A		44.892	53.709	27.900	1.00 20.00
ATOM	1965	N	GLY A		49.091	57.663	26.658	1.00 20.00
ATOM	1966	CA	GLY A		49.248	58.759	25.715	1.00 20.00
ATOM	1967	C	GLY A		48.581	60.112	25.920	1.00 20.00
ATOM	1968	ō	GLY A		48.145	60.734	24.947	1.00 20.00
ATOM	1970	N	GLY A		48.511	60.580	27.156	1.00 20.00
ATOM	1971	CA	GLY A		47.902	61.874	27.364	1.00 20.00
ATOM	1972	C	GLY A		48.981	62.925	27.245	1.00 20.00
ATOM	1973	ō	GLY A		50.097	62.697	27.759	1.00 20.00
ATOM	1975	N	THR A		48.692	64.027	26.543	1.00 20.00
ATOM	1976	CA	THR A		49.656	65.126	26.400	1.00 20.00
ATOM	1977	C	THR A		50.114	65.691	27.757	1.00 20.00
ATOM	1978	ō	THR A		49.289	65.966	28.616	1.00 20.00
ATOM	1979	CB	THR A		49.038	66.308	25.664	1.00 20.00
ATOM	1980		THR A		49.457	66.326	24.301	1.00 20.00
ATOM	1981	CG2	THR A		49.447	67.597	26.327	1.00 20.00
ATOM	1984	N	PRO A		51.445	65.866	27.966	1.00 20.00
ATOM	1985	CA	PRO A		51.925	66.416	29.237	1.00 20.00
ATOM	1986	C	PRO A		51.674	67.919	29.265	1.00 20.00
ATOM	1987	ō	PRO A		51.812	68.570	28.264	1.00 20.00
ATOM	1988	CB	PRO A		53.401	66.083	29.223	1.00 20.00
ATOM	1989	CG	PRO A		53.573	65.116	28.170	1.00 20.00
ATOM	1990	CD	PRO A		52.592	65.497	27.134	1.00 20.00
ATOM	1991	N	TYR A		51.296	68.471	30.407	1.00 20.00
ATOM	1992	CA	TYR A	039	51.040	69.900	30.494	1.00 20.00
ATOM	1993	С	TYR A		49.928	70.255	29.514	1.00 20.00
ATOM	1994	0	TYR A	039	50.174	71.011	28.551	1.00 20.00
ATOM	1995	CB	TYR A		52.317	70.678	30.156	1.00 20.00
ATOM	1996	CG	TYR A	039	53.492	70.254	31.016	1.00 20.00
ATOM	1997	CD1	TYR A	039	54.593	69.571	30.470	1.00 20.00
ATOM	1998	CD2	TYR A	039	53.456	70.437	32.381	1.00 20.00
ATOM	1999	CE1	TYR A	039	55.586	69.088	31.288	1.00 20.00
ATOM	2000	CE2	TYR A	039	54.438	69.966	33.188	1.00 20.00
ATOM	2001	CZ	TYR A	039	55.489	69.290	32.656	1.00 20.00
ATOM	2002	OH	TYR A	039	56.405	68.759	33.532	1.00 20.00
ATOM	2005	N	CYS A	040	48.713	69.706	29.757	1.00 20.00
ATOM	2006	CA	CYS A	040	47.536	69.943	28.893	1.00 20.00
ATOM	2007	С	CYS A	040	46.861	71.241	29.251	1.00 20.00
ATOM	2008	0	CYS A	040	46.426	71.456	30.371	1.00 20.00
ATOM	2009	CB	CYS A	040	46.518	68.779	28.952	1.00 20.00
ATOM	2010	SG	CYS A	040	45.587	68.439	27.332	1.00 20.00
ATOM	2012	N	GLY A	041	46.773	72.105	28.261	1.00 20.00
ATOM	2013	CA	GLY A	041	46.197	73.417	28.496	1.00 20.00
ATOM	2014	C	GLY A	041	47.251	74.257	29.222	1.00 20.00
ATOM	2015	0	GLY A	041	46.977	74.928	30.241	1.00 20.00
ATOM	2017	N	MET A	042	48.480	74.184	28.727	1.00 20.00
ATOM	2018	CA		042	49.542	74.920	29.347	1.00 20.00
ATOM	2019	C	MET A	042	50.391	75.508	28.241	1.00 20.00
ATOM	2020	0	MET A	042	50.540	74.944	27.173	1.00 20.00
ATOM	2021	CB	MET A		50.321	73.990	30.253	1.00 20.00
ATOM	2022	CG		042	50.038	74.150	31.721	1.00 20.00
MOTA	2023	SD	MET A		51.637	74.393	32.551	1.00 20.00
ATOM	2024	CE	MET A	042	51.370	73.664	34.142	1.00 20.00

 $\begin{array}{ll} \mbox{Docket/App No.:} & 2079.1037-001 \\ \mbox{Title: Method of Identifying Inhibitors of TIE-2} \\ \mbox{Inventors:} & \mbox{Nancy J. Bump et $al.} \\ \end{array}$

ATOM	2026	N	THR .	A	043		50.915	76.686	28.463	1.00 20.00
ATOM	2027	CA	THE .	A	043		51.699	77.320	27.418	1.00 20.00
ATOM	2028	С	THR .				53.137	77.204	27.856	1.00 20.00
ATOM	2029	0	THR .	A	043		53.479	77.409	29.047	1.00 20.00
ATOM	2030	CB	THR :				51.356	78.827	27.279	1.00 20.00
MOTA	2031	OG1	THR .				51.534	79.465	28.565	1.00 20.00
ATOM	2032	CG2	THR .				49.905	79.033	26.760	1.00 20.00
ATOM	2035	N	CYS .				53.977	76.862	26.885	1.00 20.00
ATOM	2036	CA	CYS :				55.388	76.714	27.139	1.00 20.00
ATOM	2037	c	CYS :				55.681	77.866	28.075	1.00 20.00
ATOM	2038	ō	CYS .				55.836	77.638	29.269	1.00 20.00
ATOM	2039	CB	CYS .				56.128	76.779	25.814	1.00 20.00
ATOM	2040	SG	CYS .				55.373	75.549	24.616	1.00 20.00
ATOM	2042	N	ALA .				55.664	79.092	27.554	1.00 20.00
MOTA	2043	CA	ALA .				55.893	80.306	28.342	1.00 20.00
MOTA	2044	c	ALA				55.536	80.155	29.809	1.00 20.00
ATOM	2045	0	ALA .				56.216	80.636	30.700	1.00 20.00
ATOM	2046	CB	ALA:				55.082	81.416	27.760	1.00 20.00
ATOM	2048	N	GLU .				54.429	79.482	30.050	1.00 20.00
ATOM	2049	CA	GLU .				53.961	79.269	31.390	1.00 20.00
ATOM	2050	c	GLU .				54.902	78.299	32.100	1.00 20.00
ATOM	2051	0	GLU .				55.309	78.558	33.243	1.00 20.00
ATOM	2052	CB	GLU .				52.556	78.738	31.281	1.00 20.00
ATOM	2053	CG	GLU .				51.601	79.002	32.429	1.00 20.00
ATOM	2054	CD	GLU .				50.437	78.036	32.341	1.00 20.00
ATOM	2055	OE1	GLU .				50.182	77.380	33.378	1.00 20.00
ATOM	2056	OE2	GLU :				49.814	77.940	31.222	1.00 20.00
ATOM	2058	N	LEU .				55.251	77.192	31.437	1.00 20.00
ATOM	2059	CA	LEU .				56.203	76.207	32.001	1.00 20.00
ATOM	2060	C	LEU .			,	57.470	76.893	32.593	1.00 20.00
ATOM	2061	0	LEU .		047		57.712	76.853	33.805	1.00 20.00
ATOM	2062	CB	LEU .		047		56.639	75.203	30.914	1.00 20.00
ATOM	2063	CG	LEU .				55.895	73.203	30.885	1.00 20.00
ATOM	2063	CD1	LEU .				56.520	72.889	29.922	1.00 20.00
ATOM	2065	CD2	LEU .				55.884	73.280	32.256	1.00 20.00
ATOM	2067	N	TYR .				58.254	77.503	31.694	1.00 20.00
ATOM	2068	CA	TYR .				59.483	78.267	31.974	1.00 20.00
ATOM	2069	C	TYR .				59.499	78.207	33.311	1.00 20.00
ATOM	2070	0	TYR				60.325	78.669	34.188	1.00 20.00
ATOM	2071	CB	TYR .				59.684	79.343	30.919	1.00 20.00
ATOM	2071	CG	TYR .				60.217	78.874	29.611	1.00 20.00
ATOM	2072	CD1	TYR				59.370	78.692	28.518	1.00 20.00
ATOM	2074	CD2	TYR				61.570	78.629	29.459	1.00 20.00
MOTA	2075		TYR				59.868	78.263	27.278	1.00 20.00
ATOM	2075	CE2	TYR				62.094	78.206	28.248	1.00 20.00
ATOM	2076	CZ.	TYR						28.248	1.00 20.00
ATOM	2077	OH	TYR				61.250 61.799	78.013 77.541	25.930	1.00 20.00
ATOM	2081	N	GLU							1.00 20.00
ATOM	2081	CA	GLU				58.601	79.954	33.446 34.680	1.00 20.00
ATOM	2082	CA					58.527	80.725		1.00 20.00
			GLU				58.074	79.756	35.720	
ATOM	2084	0	GLU				58.417	79.886	36.903	1.00 20.00
MOTA	2085	CB	GLU				57.485	81.840	34.592	1.00 20.00
MOTA	2086	CG	GLU				57.233	82.519	35.947	1.00 20.00
ATOM	2087	CD	GLU		049		55.761	82.820	36.314	1.00 20.00
ATOM	2088		GLU				54.860	82.700	35.453	1.00 20.00
ATOM	2089	OE2	GLU		049		55.540	83.185	37.497	1.00 20.00
ATOM	2091	N	LYS	Α	050		57.277	78.791	35.243	1.00 20.00

ATOM	2092	CA	LYS	A	050	56.683	77.749	36.092	1.00	20.00
ATOM	2093	С	LYS			57.625	76.655	36.652		20.00
ATOM	2094	ō	LYS			58.038	76.747	37.789		20.00
ATOM	2095	CB	LYS			55.465	77.116	35.362		20.00
ATOM	2097	N	LEU			57.965	75.640	35.880		20.00
ATOM	2098	CA	LEU			58.854	74.592	36.398		20.00
ATOM	2099	C	LEU		051	59.828	75.002	37.553		20.00
ATOM	2100	ō	LEU		051	59.835	74.350	38.608		20.00
ATOM	2101	СВ	LEU		051	59.655	73.957	35.239		20.00
ATOM	2102	CG	LEU		051	58.981	72.988	34.248		20.00
ATOM	2102	CD1	LEU		051	57.669	72.566	34.798		20.00
ATOM	2104	CD2	LEU			58.796	73.609	32.875		20.00
ATOM	2106	N	PRO			60.673	76.050	37.346		20.00
ATOM	2107	CA	PRO			61.652	76.601	38.292		20.00
ATOM	2107	C	PRO			61.323	76.418	39.750		20.00
ATOM	2109	0	PRO			61.675	75.396	40.337		20.00
ATOM		CB	PRO			61.724	78.053	37.895		20.00
	2110									20.00
ATOM	2111	CG	PRO			61.556	78.008	36.389		20.00
ATOM	2112	CD	PRO			60.771	76.762	36.051		
ATOM	2113	N	GLN			60.706	77.399	40.394		20.00
ATOM	2114	CA	GLN			60.319	77.126	41.783		20.00
ATOM	2115	C	GLN			58.915	76.531	41.498		20.00
ATOM	2116	0	GLN			58.116	76.198	42.386		20.00
ATOM	2117	CB	GLN			60.274	78.414	42.664		20.00
ATOM	2119	N	GLY			58.649	76.413	40.208		20.00
ATOM	2120	CA	GLY			57.454	75.745	39.784		20.00
ATOM	2121	C	GLY			57.520	74.261	40.190		20.00
ATOM	2122	0	GLY			58.564	73.730	40.654		20.00
ATOM	2124	N	TYR			56.363	73.629	40.002		20.00
ATOM	2125	CA	TYR			56.081	72.268	40.370		20.00
ATOM	2126	C	TYR			56.216	71.476	39.095		20.00
ATOM	2127	0	TYR			56.762	72.008	38.153		20.00
ATOM	2128	CB	TYR			54.647	72.256	40.889		20.00
ATOM	2129	CG	TYR			53.604	72.330	39.754		20.00
ATOM	2130	CD1	TYR			52.634	71.309	39.604		20.00
MOTA	2131	CD2	TYR			53.685	73.316	38.749		20.00
ATOM	2132	CE1	TYR			51.805	71.283	38.478		20.00
ATOM	2133	CE2	TYR			52.863	73.280	37.642		20.00
ATOM	2134	CZ	TYR			51.928	72.264	37.501		20.00
ATOM	2135	OH	TYR			51.114	72.171	36.375		20.00
ATOM	2138	N	ARG			55.738	70.232	39.048		20.00
MOTA	2139	CA	ARG			55.828	69.422	37.821		20.00
ATOM	2140	C	ARG			54.504	68.699	37.494		20.00
ATOM	2141	0	ARG			53.471	69.052	38.098		20.00
MOTA	2142	CB	ARG			56.926	68.379	37.948		20.00
MOTA	2143	CG	ARG			57.175	67.962	39.357		20.00
ATOM	2144	CD	ARG			58.538	68.505	39.833		20.00
MOTA	2145	NE	ARG			59.319	69.142	38.760		20.00
ATOM	2146	CZ	ARG			60.182	70.114	38.982		20.00
MOTA	2147		ARG			60.367	70.542	40.201		20.00
MOTA	2148		ARG			60.839	70.655	37.996		20.00
MOTA	2155	N	LEU			54.531	67.705	36.565		20.00
MOTA	2156	CA	LEU			53.312	66.955	36.203		20.00
ATOM	2157	C	LEU			52.643	66.257	37.370		20.00
ATOM	2158	0	LEU			53.221	65.587	38.191		20.00
MOTA	2159	CB	LEU			53.519	65.955	35.071		20.00
ATOM	2160	CG	LEU	A	057	53.850	66.384	33.632	1.00	20.00

ATOM	2161	CDl	LEU	Z.	057	54.504	65.224	32.920	1.00 20.00
ATOM	2162	CD2	LEU	A	057	52.669	66.811	32.830	1.00 20.00
ATOM	2164	N	GLU			51.357	66.515	37.390	1.00 20.00
ATOM	2165	CA	GLU			50.325	66.093	38.333	1.00 20.00
ATOM	2166	C	GLU			50.078	64.562	38.297	1.00 20.00
MOTA	2167	0	GLU .			50.013	63.978	37.216	1.00 20.00
ATOM	2168	CB	GLU .			49.091	66.872	37.885	1.00 20.00
ATOM	2169	CG	GLU .			48.798	66.637	36.334	1.00 20.00
ATOM	2170	CD	GLU .	A	058	49.565	67.548	35.341	1.00 20.00
ATOM	2171	OEl	GLU .	A	058	50.058	68.604	35.777	1.00 20.00
ATOM	2172	OE2	GLU	Α	058	49.657	67.227	34.128	1.00 20.00
ATOM	2174	N	LYS .	Α	059	49.906	63.915	39.448	1.00 20.00
ATOM	2175	CA	LYS .	Α	059	49.693	62.458	39.420	1.00 20.00
ATOM	2176	С	LYS .	A	059	48.502	61.929	38.655	1.00 20.00
ATOM	2177	ō	LYS			47.366	62.213	38.971	1.00 20.00
MOTA	2178	CB	LYS			49.607	61.825	40.814	1.00 20.00
ATOM	2179	CG	LYS			49.383	60.289	40.717	1.00 20.00
ATOM	2180	CD	LYS						1.00 20.00
						49.519	59.551	42.056	
ATOM	2181	CE	LYS .			48.286	59.754	42.979	1.00 20.00
ATOM	2182	NZ	LYS			47.400	58.540	43.161	1.00 20.00
ATOM	2187	N	PRO .			48.753	61.095	37.662	1.00 20.00
MOTA	2188	CA	PRO			47.615	60.576	36.931	1.00 20.00
ATOM	2189	C	PRO.			46.646	59.848	37.873	1.00 20.00
MOTA	2190	0	PRO			47.048	59.234	38.860	1.00 20.00
MOTA	2191	CB	PRO .	Α	060	48.260	59.643	35.923	1.00 20.00
ATOM	2192	CG	PRO	Α	060	49.662	60.187	35.751	1.00 20.00
MOTA	2193	CD	PRO .	Α	060	50.018	60.555	37.147	1.00 20.00
ATOM	2194	N	LEU .	Α	061	45.371	59.984	37.543	1.00 20.00
ATOM	2195	CA	LEU .	Α	061	44.236	59.426	38.245	1.00 20.00
MOTA	2196	C	LEU	A	061	44.496	58.098	38.924	1.00 20.00
ATOM	2197	0	LEU	A	061	44.187	57.890	40.123	1.00 20.00
ATOM	2198	CB	LEU	Α	061	43.055	59.243	37.248	1.00 20.00
ATOM	2199	CG	LEU	Α	061	42.994	59.507	35.690	1.00 20.00
ATOM	2200	CD1				44.393	59.876	35.050	1.00 20.00
ATOM	2201		LEU			42.384	58.237	35.000	1.00 20.00
ATOM	2203	N	ASN			45.075	57.203	38.117	1.00 20.00
ATOM	2204	CA	ASN			45.378	55.820	38.502	1.00 20.00
ATOM	2204	C	ASN						1.00 20.00
						46.840	55.286	38.537	
MOTA	2206	0	ASN			47.079	54.209	37.999	1.00 20.00
ATOM	2207	CB	ASN			44.591	54.958	37.559	1.00 20.00
MOTA	2208	CG	ASN			44.675	55.478	36.220	1.00 20.00
ATOM	2209		ASN			45.731	55.960	35.816	1.00 20.00
MOTA	2210	ND2				43.590	55.443	35.504	1.00 20.00
ATOM	2214	N	CYS			47.812	56.005	39.100	1.00 20.00
ATOM	2215	CA	CYS	A	063	49.165	55.418	39.205	1.00 20.00
ATOM	2216	C	CYS	A	063	49.155	55.124	40.645	1.00 20.00
ATOM	2217	0	CYS	A	063	48.285	55.550	41.377	1.00 20.00
ATOM	2218	CB	CYS	A	063	50.364	56.362	39.046	1.00 20.00
ATOM	2219	SG	CYS	A	063	50.817	56.807	37.453	1.00 20.00
ATOM	2221	N	ASP			50.186	54.449	41.067	1.00 20.00
ATOM	2222	CA	ASP			50.291	54.106	42.448	1.00 20.00
ATOM	2223	C	ASP			51.455	54.945	42.917	1.00 20.00
ATOM	2224	ō	ASP			52.521	54.903	42.319	1.00 20.00
ATOM	2225	CB	ASP			50.558	52.601	42.552	1.00 20.00
ATOM	2226	CG	ASP			50.951	52.180	43.945	1.00 20.00
ATOM	2220		7.00			50.951	52.180	43.945	1.00 20.00

COUNTRY - CHONCH

50.078 51.628 44.664 1.00 20.00

52.131 52.394 44.309 1.00 20.00

2227 OD1 ASP A 064

ATOM 2228 OD2 ASP A 064

ATOM

ATOM	2230	N	ASP A		51.259	55.718	43.973	1.00 20.00
ATOM	2231	CA	ASP A		52.332	56.577	44.460	1.00 20.00
ATOM	2232	C	ASP A		53.733	56.051	44.341	1.00 20.00
MOTA	2233	0	ASP A		54.642	56.B60	44.332	
MOTA	2234	CB	ASP A		52.062	57.029	45.875	1.00 20.00
MOTA	2235	CG	ASP A		50.937	58.020	45.923	1.00 20.00
MOTA	2236		ASP A		50.842	58.814	44.958	1.00 20.00
MOTA	2237		ASP A		50.136	58.013	46.883	1.00 20.00
MOTA	2239	N	GLU A		53.918	54.734	44.222	1.00 20.00
MOTA	2240	CA	GLU A		55.255	54.179	44.049	1.00 20.00
ATOM	2241	С	GLU A		55.670	54.466 54.554	42.600	1.00 20.00
ATOM	2242	0	GLU A		56.854	52.656	44.363	1.00 20.00
ATOM	2243	CB	GLU A		55.315			1.00 20.00
ATOM	2244	CG	GLU A		54.520	52.182	45.635 46.237	1.00 20.00
ATOM	2245	CD	GLU A		54.944 54.716	50.804	47.469	1.00 20.00
ATOM	2246	OE1	GLU A			49.937	45.496	1.00 20.00
ATOM	2247	OE2	GLU A		55.494		41.671	1.00 20.00
MOTA	2249	N	VAL A		54.726	54.592	40.293	1.00 20.00
MOTA	2250	CA	VAL A		55.092 55.224	54.941 56.462	40.293	1.00 20.00
ATOM	2251	C				56.986	39.410	1.00 20.00
ATOM	2252	0	VAL A		56.000	54.487	39.279	1.00 20.00
ATOM	2253	CB	VAL A		54.055		37.857	1.00 20.00
ATOM	2254	CG1	VAL A		54.600	54.593	39.597	1.00 20.00
ATOM	2255	CG2	VAL A		53.657	53.116	40.948	1.00 20.00
ATOM	2257	N	TYR A		54.460 54.614	57.189 58.609	40.861	1.00 20.00
MOTA	2258	CA	TYR A				41.455	1.00 20.00
ATOM	2259	C	TYR A		55.973	59.018	40.831	1.00 20.00
ATOM	2260	0	TYR A		56.712	59.819	41.595	1.00 20.00
ATOM	2261	CB	TYR A		53.489 53.361	59.313 60.752	41.220	1.00 20.00
ATOM	2262		TYR A		53.361	61.124	39.920	1.00 20.00
MOTA	2263	CD1 CD2	TYR F		53.490	61.746	42.186	1.00 20.00
ATOM	2264		TYR F		53.490	62.478	39.603	1.00 20.00
ATOM	2265	CE1	TYR F		53.395	63.060	41.887	1.00 20.00
ATOM	2266		TYR A		53.393	63.435	40.612	1.00 20.00
MOTA	2267	CZ OH	TYR A		53.171	64.768	40.328	1.00 20.00
ATOM	2268	N		069	56.315	58.503	42.647	1.00 20.00
ATOM	2271	CA		069	57.609	58.859	43.214	1.00 20.00
ATOM	2272	C	ASP A		58,773	58.615	42.263	1.00 20.00
ATOM ATOM	2273 2274	0		069	59.744	59.344	42.299	1.00 20.00
ATOM	2275	CB	ASP A		57.969	58.107	44.464	1.00 20.00
ATOM	2275	CG	ASP I		59.422	58.423	44.879	1.00 20.00
ATOM	2277		ASP I		60.352	57.615	44.540	1.00 20.00
MOTA	2278	OD2			59.635	59.510	45.509	1.00 20.00
ATOM	2280	N	LEU /		58.720	57.565	41.452	1.00 20.00
ATOM	2280	CA	LEU A		59.809	57.334	40.528	1.00 20.00
ATOM	2282	C	LEU A		59.790	58.516	39.558	1.00 20.00
ATOM	2283	0	LEU A		50.802	59.127	39.276	1.00 20.00
ATOM	2284	CB	LEU A		59.609	56.013	39.765	1.00 20.00
MOTA	2285	CG	LEU A		60.747	55.706	38.780	1.00 20.00
ATOM	2286	CD1			61.879	55.168	39.574	1.00 20.00
	2286		LEU		60.351	54.769	37.681	1.00 20.00
ATOM	2287	N N		A 071	58.597	58.816	39.073	1.00 20.00
ATOM ATOM	2299	CA		a 071	58.336	59.892	38.116	1.00 20.00
ATOM	2290	CA	MET		59.004	61.168	38.549	1.00 20.00
ATOM	2291	0		A 071	59.698	61.796	37.776	1.00 20.00
	2292	CB		A 071	56.818	60.169	38.000	1.00 20.00
MOTA	2293	CB	PILL .	. 0/1	20.010	00.100	50.000	

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			MET A	077	56.219	59.904	36.636	1.00 20.00
ATOM	2294	CG			54.409	59.761	36.764	1.00 20.00
ATOM	2295	SD		071	53.977	58.683	35.467	1.00 20.00
ATOM	2296	CE		071			39.803	1.00 20.00
MOTA	2298	N	ARG A		58.797	61.527 62.762	40.345	1.00 20.00
MOTA	2299	CA	ARG A		59.303		40.778	1.00 20.00
MOTA	2300	C	ARG A		60.739	62.807	40.778	1.00 20.00
ATOM	2301	0		072	61.312	63.884	41.499	1.00 20.00
MOTA	2302	CB	ARG A		58.412	63.145		1.00 20.00
MOTA	2303	CG	ARG A		56.978	63.140	41.074	1.00 20.00
ATOM	2304	CD		072	56.500	64.539	41.064	1.00 20.00
MOTA	2305	NE	ARG A		56.642	65.063	42.415	1.00 20.00
MOTA	2306	CZ	ARG A		56.484	66.337	42.720	
ATOM	2307		ARG A		56.181	67.175	41.753	1.00 20.00
MOTA	2308		ARG A		56.642	66.771	43.968	1.00 20.00
MOTA	2315	N	GLN A		61.325	61.647	41.011	1.00 20.00
ATOM	2316	CA	GLN A		62.717	61.652	41.387	1.00 20.00
ATOM	2317	C	GLN A		63.481	61.931	40.084	1.00 20.00
ATOM	2318	0	GLN A		64.658	62.267	40.105	1.00 20.00
ATOM	2319	CB	GLN P		63.124	60.316	41.973	1.00 20.00
MOTA	2320	CG	GLN A		63.076	60.211	43.490	1.00 20.00
ATOM	2321	CD	GLN A		63.603	58.852	43.962	1.00 20.00
ATOM	2322	OE1			63.853	58.641	45.159	1.00 20.00
ATOM	2323	NE2	GLN P		63.792	57.925	43.008	1.00 20.00
ATOM	2327	N	CYS F		62.819	61.805	38.947	1.00 20.00
ATOM	2328	CA	CYS F	074	63.503	62.093	37.720	1.00 20.00
ATOM	2329	C		074	63.403	63.601	37.500	1.00 20.00
ATOM	2330	0	CYS 7		64.073	64.148	36.642	1.00 20.00
ATOM	2331	CB	CYS F	074	62.847	61.361	36.524	1.00 20.00
ATOM	2332	SG	CYS A		62.746	59.548	36.564	1.00 20.00
ATOM	2334	N	TRP A		62.555	64.268	38.277	1.00 20.00
ATOM	2335	CA	TRP A		62.311	65.708	38.110	1.00 20.00
ATOM	2336	C	TRP A	075	62.906	66.552	39.231	1.00 20.00
ATOM	2337	0	TRP A	075	62.503	67.692	39.466	1.00 20.00
ATOM	2338	CB	TRP A	075	60.79 7	65.977	38.037	1.00 20.00
MOTA	2339	CG	TRP A	075	60.090	65.403	36.830	1.00 20.00
ATOM	2340	CD1	TRP A	075	60.586	65.308	35.565	1.00 20.00
MOTA	2341	CD2	TRP A	075	58.768	64.834	36.789	1.00 20.00
ATOM	2342	NE1	TRP A	075	59.669	64.720	34.751	1.00 20.00
ATOM	2343	CE2	TRP A	075	58.542	64.416	35.468	1.00 20.00
ATOM	2344	CE3	TRP A	075	57.755	64.634	37.742	1.00 20.00
ATOM	2345	CZ2	TRP A	075	57.343	63.808	35.062	1.00 20.00
ATOM	2346	CZ3	TRP A	1 075	56.551	64.024	37.331	1.00 20.00
MOTA	2347	CH2	TRP A	075	56.366	63.624	36.002	1.00 20.00
ATOM	2350	N	ARG A	076	63.865	65.959	39.934	1.00 20.00
ATOM	2351	CA	ARG A	A 076	64.533	66.625	41.024	1.00 20.00
ATOM	2352	C	ARG 2	076	65.304	67.793	40.364	1.00 20.00
ATOM	2353	0	ARG 2	4 076	65.983	67.586	39.347	1.00 20.00
ATOM	2354	CB	ARG 2	076	65.462	65.607	41.699	1.00 20.00
MOTA	2355	CG	ARG 2	A 076	64.890	64.932	42.981	1.00 20.00
MOTA	2356	CD	ARG 2	A 076	65.230	63.413	43.072	1.00 20.00
ATOM	2357	NE	ARG :	4 076	64.997	62.813	44.416	1.00 20.00
ATOM	2358	CZ	ARG :	A 076	65.490	61.630	44.835	1.00 20.00
MOTA	2359	NHl	ARG :	A 076	66.258	60.880	44.037	1.00 20.00
ATOM	2360	NH2	ARG .	A 076	65.231	61.211	46.069	1.00 20.00
ATOM	2367	N	GLU .	4 077	65.178	69.014	40.895	1.00 20.00
ATOM	2368	CA	GLU .	A 077	65.885	70.155	40.318	1.00 20.00
ATOM	2369	C	GLU .	A 077	67.310	69.773	39.983	1.00 20.00

Docket/App No.: 2079.1037-001 Title: Method of Identifying Inhibitors of TIE-2

Nancy J. Bump et al.

ATOM 2370 0 GLU A 077 67.613 69.364 38.878 1.00 20.00 MOTA 2371 CB GLU A 077 65.889 71.343 41.278 1.00 20.00 ATOM 2373 N LYS A 078 68.184 69.910 40.953 1.00 20.00 ATOM 2374 CA LYS A 078 69.573 69.583 40.764 1.00 20.00 MOTA 2375 C LYS A 078 69.811 68.228 40.037 1.00 20.00 2376 0 ATOM LYS A 078 69.850 67.194 40.664 1.00 20.00 MCTA 2377 CB LYS A 078 70.225 69.573 42.138 1.00 20.00 ATOM 2378 CG LYS A 078 69.346 70.070 43.275 1.00 20.00 ATOM 2379 CD LYS A 078 70.069 69.962 44.591 1.00 20.00 70.069 69.962 44.591 1.00 20.00 69.301 70.580 45.713 1.00 20.00 69.362 69.789 47.005 1.00 20.00 70.261 66.980 38.021 1.00 20.00 70.261 66.980 38.006 1.00 20.00 ATOM 2380 CE LYS A 078 ATOM 2381 NZ LYS A 078 ATOM 2386 N PRO A 079 2367 CA PRO A 079 MOTA 70.261 66.980 38.006 1.00 20.00 ATOM 2388 C PRO A 079 70.943 65.885 38.771 1.00 20.00 ATOM 2389 0 PRO A 079 70.451 64.770 38.811 1.00 20.00 2389 O PRO A 079 2390 CB PRO A 079 2391 CG PRO A 079 2392 CD PRO A 079 2393 N TYR A 080 ATOM 71.059 67.370 36.772 1.00 20.00 MOTA 70.896 68.782 36.633 1.00 20.00 ATOM 70.218 69.385 37.832 1.00 20.00 ATOM 72.085 66.172 39.382 1.00 20.00 2394 CA TYR A 080 ATOM 72.804 65.132 40.133 1.00 20.00 ATOM 2395 C TYR A 080 71.975 64.531 41.286 1.00 20.00 ATOM 2396 O TYR A 080 72.444 63.680 42.014 1.00 20.00 ATOM 2397 CB TYR A 080 74.139 65.707 40.640 1.00 20.00 ATOM 2398 CG TYR A 080 74.006 66.804 41.677 1.00 20.00 ATOM 2399 CD1 TYR A 080 74.086 66.521 43.022 1.00 20.00 MOTA 2400 CD2 TYR A 080 73.757 68.117 41.304 1.00 20.00 ATOM 2401 CE1 TYR A 080 73.915 67.500 43.955 1.00 20.00 ATOM 2402 CE2 TYR A 080 73.588 69.104 42.245 1.00 20.00 73.664 68.784 43.562 1.00 20.00 73.475 69.749 44.512 1.00 20.00 70.743 65.007 41.436 1.00 20.00 ATOM 2403 CZ TYR A 080 2404 OH TYR A 080 MOTA ATOM 2407 N GLU A 081 ATOM 2408 CA GLU A 081 69.817 64.540 42.462 1.00 20.00 ATOM 2409 C GLU A 081 68.878 63.538 41.797 1.00 20.00 2410 0 ATOM GLU A 081 68.205 62.751 42.451 1.00 20.00 2411 CB GLU A 081 2412 CG GLU A 081 ATOM 69.025 65.709 43.038 1.00 20.00 69.358 66.053 44.505 1.00 20.00 ATOM 2413 CD GLU A 081 ATOM 68.385 67.067 45.106 1.00 20.00 ATOM 2414 OE1 GLU A 081 68.518 67.413 46.316 1.00 20.00 ATOM 2415 OE2 GLU A 081 67.485 67.510 44.342 1.00 20.00 ATOM 2417 N ARG A 082 68.875 63.582 40.471 1.00 20.00 ATOM 2418 CA ARG A 082 68.097 62.678 39.655 1.00 20.00 ATOM 2419 C ARG A 082 68.622 61.223 39.710 1.00 20.00 69.814 60.963 39.981 1.00 20.00 68.085 63.174 38.218 1.00 20.00 66.784 63.856 37.837 1.00 20.00 ATOM 2420 O ARG A 082 ATOM 2421 CB ARG A 082 2422 CG ARG A 082 ATOM 2423 CD ARG A 082 ATOM 66.836 65.398 37.781 1.00 20.00 67.235 65.968 36.451 1.00 20.00 67.427 67.194 36.163 1.00 20.00 67.285 68.107 37.101 1.00 20.00 67.805 67.552 34.947 1.00 20.00 67.725 60.237 39.513 1.00 20.00 68.223 58.866 to sex ATOM 2424 NE ARG A 082 ATOM 2425 CZ ARG A 082 ATOM 2426 NH1 ARG A 082 2427 NH2 ARG A 082 ATOM 2434 N ATOM PRO A 083 ATOM 2435 CA PRO A 083 2436 C PRO A 083 ATOM 69.042 58.596 38.310 1.00 20.00 ATOM 2437 0 PRO A 083 69.594 59.505 37.688 1.00 20.00 2438 CB PRO A 083 65.842 58.037 39.582 1.00 20.00 2439 CG PRO A 083 65.877 58.981 40.016 1.00 20.00 ATOM ATOM ATOM 2440 CD PRO A 083

66.265 60.243 39.330 1.00 20.00

ATOM	2441	N	SFI	ה כ	084	69.	210	57.327	37.952		
ATOM	2442	CA			084	69.		56.896			20.00
ATOM	2443	C			. 084	69.		55.647	36.760		20.00
ATOM	2444	Ö			084	68.		54.760	36.225 36.990	1.00	
ATOM	2445	CB			084	71.		56.583		1.00	
ATOM	2446	OG			084	71.		55.714	37.087 38.182	1.00	20.00
ATOM	2449	N			085	69.		55.585		1.00	
ATOM	2450	CA			085	68.		54.457	34.905 34.249	1.00	
ATOM	2451	C	PHE		085	68.		53.087	34.761	1.00	
ATOM	2452	ō	PHE		085	68.		52.089	34.478		20.00
ATOM	2453	CB			085	68.		54.555	32.762		20.00
ATOM	2454	CG	PHE		085	68.		55.805	32.170		20.00
ATOM	2455	CD1			085	68.		56.546	31.303	1.00	20.00
ATOM	2456	CD2			085	66.		56.277	32.507		20.00
ATOM	2457	CE1			085	68.		57.738	30.784		20.00
ATOM	2458	CE2			085	66.		57.456	31.995		20.00
ATOM	2459	CZ			085	67.		58.174	31.140		20.00
ATOM	2461	N			086	69.		53.030	35.509		20.00
ATOM	2462	CA			086	70.		51.757	35.993		20.00
ATOM	2463	C			086	69.		51.422	37.206		20.00
ATOM	2464	ō			086	69.1		50.291	37.352		20.00
ATOM	2465	CB			086	71.		51.807	36.323		20.00
ATOM	2467	N			087	69.3		52.398	38.071		20.00
ATOM	2468	CA			087	68.4		52.121	39.266		20.00
ATOM	2469	C			087	66.		52.163	39.068		20.00
ATOM	2470	ō			087	66.		51.560	39.846		20.00
ATOM	2471	CB			087	68.5		53.074	40.388		20.00
ATOM	2472	CG			087	69.5		54.391	39.973		20.00
ATOM	2473	CD			087	70.3		55.057	41.121		20.00
ATOM	2474	OE1	GLN	Α	087	71.		56.032	40.897		20.00
MOTA	2475	NE2	GLN	A	087	70.2		54.536	42.341		20.00
ATOM	2479	N	ILE	A	088	66.5		52.883	38.025		20.00
ATOM	2480	CA	ILE	Α	088	65.1		53.054	37.686		20.00
ATOM	2481	C	ILE	Α	088	64.6		51.697	37.241		20.00
ATOM	2482	0	ILE	Α	880	63.6		51.196	37.639		20.00
ATOM	2483	CB	ILE	Α	088	64.5		54.057	36.496		20.00
MOTA	2484	CG1	ILE	Α	088	64.7	69	55.490	37.007		20.00
ATOM	2485	CG2	ILE	Α	088	63.7	29	53.684	35.655		20.00
ATOM	2486	CD1	ILE	A	088	65.3		56.556	36.035		20.00
MOTA	2488	N	LEU	Α	089	65.5	15	51.128	36.379		20.00
ATOM	2489	CA	LEU	Α	089	65.3		49.789	35.843		20.00
ATOM	2490	C	LEU	Α	089	65.0	60 -	48.826	36.994		20.00
ATOM	2491	0	LEU	Α	089	64.0	18 4	48.175	37.061		20.00
ATOM	2492	CB	LEU	A	089	66.5	40	19.336	35.092	1.00	20.00
ATOM	2493	CG	LEU	Α	089	66.5		17.848	34.823		20.00
MOTA	2494	CD1	LEU	A	089	65.1	47	17.379	34.407		20.00
MOTA	2495	CD2	LEU	Α	089	67.5	45	27.575	33.708		20.00
ATOM	2497	N	VAL	A	090	66.0	04	48.748	37.908	1.00	20.00
ATOM	2498	CA	VAL	Α	090	65.8	21 4	17.903	39.051	1.00	20.00
ATOM	2499	C	VAL		090	64.5		8.276	39.816	1.00	20.00
ATOM	2500	0	VAL		090	64.2	76 4	7.684	40.843	1.00	20.00
ATOM	2501	CB	VAL		090	66.9		18.040	39.968	1.00	20.00
ATOM	2502	CGl	VAL		090	66.5		8.001	41.390	1.00	20.00
MOTA	2503	CG2	VAL		090	68.0		6.942	39.655	1.00	20.00
ATOM	2505	N	SER		091	63.8		9.232	39.295	1.00	20.00
ATOM	2506	CA	SER			62.6		9.777	39.990	1.00	20.00
ATOM	2507	C	SER	А	091	61.2	24 4	9.394	39.462	1.00	20.00

ATOM	2508	0	SER	А	091	60.265	49.286	40.228	1.00 20.00
ATOM	2509	CB	SER	A	091	62.780	51.317	40.030	1.00 20.00
ATOM	2510	O.C	SER		091	63.064	51.756	41.334	1.00 20.00
ATOM	2513	N	LEU		092	61.125	49.264	38.146	1.00 20.00
ATOM	2514	CA	LEU	А	092	59.906	48.874	37.485	1.00 20.00
ATOM	2515	C	LEU	А	092	59.997	47.345	37.496	1.00 20.00
ATOM	2516	0	LEU	Α	092	58.987	46.643	37.662	1.00 20.00
ATOM	2517	CB	LEU		092	59.941	49.394	36.065	1.00 20.00
ATOM	2518	CG	LEU	Α	092	60.797	50.625	35.992	1.00 20.00
ATOM	2519	CD1	LEU			60.882	51.169	34.601	1.00 20.00
ATOM	2520	CD2	LEU		092	60.174	51.616	36.871	1.00 20.00
ATOM	2522	N	ASN		093	61.243	46.886	37.306	1.00 20.00
ATOM	2523	CA	ASN			61.699	45.495	37.299	1.00 20.00
ATOM	2524	C	ASN		093	61.214	44.889	38.582	1.00 20.00
ATOM	2525	0	ASN			60.803	43.724	38.635	1.00 20.00
ATOM	2526	CB	ASN			63.206	45.466	37.438	1.00 20.00
ATOM	2527	CG	ASN	A	093	63.927	44.920	36.244	1.00 20.00
ATOM	2528	OD1	ASN			65.126	44.666	36.350	1.00 20.00
ATOM	2529	ND2	ASN	A	0.93	63.245	44.739	35.117	1.00 20.00
ATOM	2533	N	ARG			61.344	45.693	39.631	1.00 20.00
ATOM	2534	CA	ARG			60.992	45.309	40.985	1.00 20.00
ATOM	2535	C	ARG			59.515	45.614	41.318	1.00 20.00
ATOM	2536	ō	ARG			59.112	45.717	42.468	1.00 20.00
ATOM	2537	CB	ARG			61.954	46.010	41.937	1.00 20.00
ATOM	2538	CG	ARG			61.850	45.571	43.339	1.00 20.00
ATOM	2539	CD	ARG			62.088	46.747	44.262	1.00 20.00
ATOM	2540	NE	ARG			61.170	46.917	45.403	1.00 20.00
ATOM	2541	CZ	ARG			59.842	47.007	45.328	1.00 20.00
ATOM	2542	NH1	ARG			59.224	46.948	44.164	1.00 20.00
ATOM	2543	NH2	ARG			59.129	47.209	46.438	1.00 20.00
ATOM	2550	N	MET	Α	095	58.710	45.750	40.278	1.00 20.00
ATOM	2551	CA	MET	А	095	57.306	46.018	40.421	1.00 20.00
ATOM	2552	C	MET	A	095	56.723	44.944	39.527	1.00 20.00
ATOM	2553	0	MET	А	095	55.597	44.512	39.706	1.00 20.00
ATOM	2554	CB	MET	Α	0.95	56.967	47.406	39.870	1.00 20.00
ATOM	2555	CG			095	57.240	48.556	40.822	1.00 20.00
ATOM	2556	SD	MET	А	095	56.618	50.279	40.365	1.00 20.00
ATOM	2557	CE	MET	Α	095	56.509	50.955	42.056	1.00 20.00
MCTA	2559	N	LEU	А	096	57.495	44.509	38.551	1.00 20.00
ATOM	2560	CA	LEU	Α	096	57.034	43.476	37.646	1.00 20.00
ATOM	2561	C	LEU	Α	096	56.931	42.034	38.341	1.00 20.00
ATOM	2562	0	LEU	Α	096	56.594	40.999	37.738	1.00 20.00
ATOM	2563	CB	LEU	А	096	57.960	43.493	36.401	1.00 20.00
ATOM	2564	CG	LEU	Α	096	57.892	44.684	35.421	1.00 20.00
ATOM	2565	CD1	LEU	Α	096	58.856	44.515	34.311	1.00 20.00
ATOM	2566	CD2	LEU	А	096	56.523	44.804	34.819	1.00 20.00
ATOM	2568	И	GLU	Α	097	57.181	41.981	39.633	1.00 20.00
ATOM	2569	CA	GLU	A	097	57.102	40.734	40.327	1.00 20.00
ATOM	2570	C	GLU	Α	097	56.396	40.934	41.642	1.00 20.00
ATOM	2571	0	GLU	Α	097	57.064	41.042	42.664	1.00 20.00
ATOM	2572	CB	GLU	A	097	58.499	40.252	40.606	1.00 20.00
ATOM	2573	CG	ĞLU	А	097	59.459	40.519	39.475	1.00 20.00
ATOM	2574	CD	GLU	Α	097	60.327	39.305	39.212	1.00 20.00
MOTA	2575	OE1	GLU	Α	097	60.756	38.703	40.228	1.00 20.00
MOTA	2576	OE2	GLU	Α	097	60.564	38.961	38.022	1.00 20.00
ATOM	2578	N	GLU	Α	098	55.062	41.010	41.622	1.00 20.00
MOTA	2579	CA	GLU	A	098	54.192	41.177	42.823	1.00 20.00

ATOM	2580	С	GLH	2	098	52.812	41.404	42.219	7 00	20.00
ATOM	2581	0	GLU		098	51.765	41.462	42.905		20.00
ATOM	2582	CB		A	098	54.514	42.433	43.686		20.00
ATOM	2583	CG	GLU	A	098	55.726	43.286	43.421		20.00
ATOM	2584	CD	GLU	A	098	56.655	43.318	44.654		20.00
ATOM	2585	OE1	GLU	Α	098	56.157	43.414	45.803		20.00
ATOM	2586	OE2	GLU		098	57.903	43.232	44.488		20.00
ATOM	2588	N	ARG		099	52.872	41.529	40.898		20.00
ATOM	2589	CA	ARG		099	51.725	41.820	40.069		20.00
ATOM	2590	C	ARG		099	50.664	42.484	40.859		20.00
ATOM	2591	0	ARG		099	49.536	41.992	40.833		20.00
ATOM	2592	CB	ARG		099	51.107	40.600	39.385		20.00
ATOM	2593	CG			099	50.252				20.00
ATOM	2594	CD	ARG			49.462	41.009	38.173		20.00
ATOM	2595	NE	ARG			48.780	42.327 42.813	38.402 37.193		20.00
ATOM	2596	CZ			099	48.995	44.001	36.614		20.00
ATOM	2597	NH1	ARG			49.888	44.858	37.132		20.00
ATOM	2598	NH2	ARG			48.348				20.00
ATOM	2605	N	LYS		100	51.012	44.319	35.492		
ATOM	2606	CA			100		43.593	41.491		20.00
ATOM	2607	C	LYS			49.996	44.273	42.208		20.00
ATOM	2608	0	LYS			49.233	45.314	41.412		20.00
ATOM	2609	CB	LYS		100	48.414	46.009	41.961		20.00
ATOM	2610	CG	LYS			50.568	44.887	43.452		20.00
ATOM	2611	CD	LYS			49.723	44.455	44.606		20.00
MOTA		CE	LYS			48.746	43.295	44.135		20.00
MOTA	2612 2613	NZ	LYS			47.476	43.250	44.951		20.00
ATOM	2618	N	THR			47.799 49.448	42.986	46.386		20.00
ATOM	2619	CA	THR			48.825	45.372	40.107		20.00
ATOM	2620	C	THR		101		46.402	39.284		20.00
ATOM	2621	0	THR			49.208 48.788	47.748 48.131	39.873 40.984		20.00
ATOM	2622	CB	THR			47.325				20.00
ATOM	2623	OG1	THR			46.859	46.313 45.424	39.223 40.224		20.00
ATOM	2624	CG2	THR			46.913	45.840	37.852		20.00
ATOM	2627	N	TYR			50.025	48.453			20.00
ATOM	2628	CA	TYR			50.547	49.712	39.098 39.515		20.00
ATOM	2629	C	TYR			49.870	50.826	38.785		20.00
ATOM	2630	0	TYR			49.661	51.891	39.342		20.00
ATOM	2631	CB	TYR			52.040	49.684	39.342		20.00
ATOM	2632	CG	TYR			52.744	49.084	40.406		20.00
ATOM	2633	CD1	TYR			53.416	47.744	40.400	1.00	
ATOM	2634	CD2	TYR			52.769		41.663	1.00	
ATOM	2635	CEI	TYR			54.090	49.460 47.122	41.160		20.00
ATOM	2636	CE2	TYR			53.430	48.852	42.653		20.00
ATOM	2637	CZ	TYR			54.102				
ATOM	2638	OH	TYR			54.846	47.691	42.416	1.00	
ATOM	2641	N	VAL			49.568	47.188 50.591	43.470 37.524	1.00	20.00
ATOM	2642	CA	VAL		103	48.790	51.544	36.741		20.00
ATOM	2643	C	VAL		103					
ATOM	2644	0	VAL		103	47.512 47.571	50.735 49.547	36.788 37.137	1.00	20.00
ATOM	2645	CB	VAL			49.121	51.597	35.265		20.00
ATOM	2646	CG1	VAL		103	48.387	52.783	34.645		20.00
ATOM	2647	CG2	VAL		103	50.633	51.634	35.049	1.00	
ATOM	2649	N N	ASN		103	46.380	51.834	36.420		20.00
ATOM	2650	CA	ASN		104	45.109	50.645	36.420		20.00
ATOM	2651	C	ASN		104	44.386	51.023	35.231		20.00
ATOM	2652	0	ASN		104	44.569	52.110	34.731		20.00
		~	* JOH		~ レス	TT. JOJ	U	J t . / J L	1.00	20.00

ATOM	2653	CB	ASN I	104	44.360	51.089	37.714	1.00 20.00
ATOM	2654	CG	ASN A		42.863	51.071	37.544	1.00 20.00
ATOM	2655		ASN A		42.348	51.013	36.431	1.00 20.00
ATOM	2656	ND2	ASN A		42.149	51.139	38.666	1.00 20.00
ATOM	2660	N	THR A		43.545	50.137	34.732	1.00 20.00
ATOM	2661	CA	THR A		42.855	50.390	33.490	1.00 20.00
ATOM	2662	c	THR A		41.412	49.870	33.596	1.00 20.00
ATOM	2663	0	THR A		40.678	49.783	32.593	1.00 20.00
ATOM	2664	CB	THR A		43.627	49.686	32.341	1.00 20.00
ATOM	2665	OG1	THR A		44.293	48.501	32.839	1.00 20.00
ATOM	2666	CG2	THR A		44.686	50.595	31.792	1.00 20.00
ATOM	2669	N	THR A		41.013	49.565	34.831	1.00 20.00
ATOM	2670	CA	THR A		39.701	49.048	35.173	1.00 20.00
ATOM	2671	C	THR A		38.588	50.103	35.353	1.00 20.00
ATOM	2672	0	THR A		38.818	51.077	36.038	1.00 20.00
MOTA	2673	CB	THR A		39.850	48.258	36.473	1.00 20.00
ATOM	2674	OG1	THR A		39.615		36.226	1.00 20.00
ATOM	2675	CG2	THR A			46.869	36.226	
ATOM	2678	N	LEU A		38.902	48.779		1.00 20.00
ATOM	2679	CA	LEU A		37.383 36.229	49.891	34.775 34.903	1.00 20.00
ATOM	2680	C	LEU A		35.437	50.816		
ATOM	2681	0	LEU 1		35.437	50.546 49.413	36.199 36.473	1.00 20.00
ATOM	2682	CB	LEU 1					
ATOM	2683	CG	LEU A		35.279	50.655	33.739	1.00 20.00
ATOM	2684		LEU !		35.798	50.744	32.313	1.00 20.00
ATOM	2685		LEU A		34.625	50.728	31.345	1.00 20.00
ATOM	2685	N				51.987	32.120	1.00 20.00
ATOM	2688	CA	TYR I			51.583	36.998	1.00 20.00
ATOM	2689	C	TYR A		34.436	51.444	38.260	1.00 20.00
ATOM	2690	0	TYR A		33.529	52.660	38.590	1.00 20.00
ATOM	2691	CB	TYR A		33.124	52.843	39.767	1.00 20.00
ATOM	2691	CG	TYR /		35.417 36.234	51.219	39.419	1.00 20.00
ATOM	2693	CD1	TYR A			49.960	39.165	1.00 20.00
ATOM	2694	CD2	TYR 3		37.446	49.725	40.176	1.00 20.00
ATOM	2696	N N	GLU A			48.850	39.201	1.00 20.00
ATOM	2697	CA	GLU 1		33.228	53.475	37.565	1.00 20.00
ATOM	2698	C	GLU A		32.363	54.664	37.691	1.00 20.00
ATOM	2699	0	GLU A		33.115	55.935	37.364	1.00 20.00
ATOM	2700	CB	GLU A		34.039 31.764	56.360 54.786	38.093	1.00 20.00
ATOM	2702	N	LYS A				39.092	1.00 20.00
ATOM	2703	CA	LYS A		32.723 33.431	56.590	36.284	1.00 20.00
ATOM	2704	C	LYS !			57.801	35.968	1.00 20.00
MOTA	2705	0	LYS A		34.879	57.443	35.586	1.00 20.00
ATOM	2706	CB	LYS A		35.653 33.373	56.902 58.742	36.366	1.00 20.00
ATOM	2707	CG	LYS 3		32.211	58.399	37.176	1.00 20.00
ATOM	2708	CD	LYS A				38.165	1.00 20.00
ATOM	2709	CE	LYS 2		31.414 30.154	59.597		
ATOM	2710	NZ	LYS 2			59.092	39.514	1.00 20.00
ATOM	2715	N	PHE I		30.320	58.678	40.967	1.00 20.00
ATOM	2716	CA	PHE A		35.184	57.675	34.324	1.00 20.00
ATOM	2717	C	PHE A		36.489	57.460	33.833	
ATOM	2717	0	PHE P		36.665	58.179	32.520	1.00 20.00
ATOM	2719	CB			36.065	57.840	31.494	1.00 20.00
ATOM	2719	CG	PHE A		36.842	55.994	33.658	1.00 20.00
ATOM	2721	CD1	PHE A		38.193	55.795	33.013	1.00 20.00
ATOM	2721	CD2			39.337	55.675	33.772	1.00 20.00
ATOM	2723				38.332	55.861	31.657	1.00 20.00
ELL OUT	2123	CE1	PHE A	4 4 4 4	40.601	55.639	33.171	1.00 20.00

ATOM	2724	CE2	PHE A	111	39.575	55.824	31.077	1.00	20.00
ATOM	2725	CZ	PHE A		40.706	55.717	31.830		20.00
ATOM	2727	N	THR A		37.540	59.180	32.584	1.00	
ATOM	2728	CA	THR A		37.904	59.997	31.457	1.00	
ATOM	2729	C	THR A		39.374	59.703	31.350	1.00	
ATOM	2730	0	THR A		39.967	59.297	32.329	1.00	
ATOM		CB	THR A						
	2731				37.686	61.487	31.794	1.00	
ATOM	2732	OG1 CG2	THR A		36.780	61.598	32.899	1.00	
ATOM	2733		THR A		37.079	62.216	30.623		20.00
ATOM	2736	N	TYR A		39.926	59.880	30.153	1.00	
ATOM	2737	CA	TYR A		41.339	59.706	29.866		20.00
ATOM	2738	С	TYR A		42.092	61.000	30.123	1.00	
ATOM	2739	0	TYR A		41.837	61.669	31.105		20.00
ATOM	2740	CB	TYR A		41.520	59.320	28.433		20.00
ATOM	2741	CG	TYR A		41.095	57.923	28.236		20.00
ATOM	2742	CD1	TYR A		40.063	57.606	27.346	1.00	20.00
ATOM	2743	CD2	TYR A	113	41.699	56.879	28.960	1.00	20.00
MOTA	2744	CE1	TYR A	113	39.641	56.300	27.178	1.00	20.00
ATOM	2745	CE2	TYR A	113	41.283	55.573	28.792	1.00	20.00
ATOM	2746	CZ	TYR A	113	40.251	55.291	27.894	1.00	20.00
ATOM	2747	OH	TYR A	113	39.853	53.992	27.670	1.00	20.00
ATOM	2750	N	ALA A	114	42.958	61.423	29.201	1.00	20.00
ATOM	2751	CA	ALA A	114	43.754	62.605	29.511		20.00
ATOM	2752	C	ALA A		43.947	63.838	28.571		20.00
ATOM	2753	ō	ALA A		43.604	64.944	28.952		20.00
ATOM	2754	CB	ALA A		45.129	62.109	30.025		20.00
ATOM	2756	N	GLY A		44.491	63.670	27.377		20.00
ATOM	2757	CA	GLY A		44.727	64.815	26.532		20.00
ATOM	2758	C	GLY A		44.350	64.834	25.059		20.00
ATOM	2759	0	GLY A		45.029	64.291	24.173		20.00
ATOM	2761	N	ILE A						
ATOM	2762	CA	ILE A		43.220	65.504	24.838		20.00
ATOM	2763		ILE A		42.609	65.779	23.527		20.00
		C			41.516	64.772	23.037		20.00
ATOM	2764	0	ILE A		41.123	63.952	23.880	1.00	
ATOM	2765	CB	ILE A		43.744	65.993	22.469	1.00	
ATOM	2766	OXT	ILE A	116	41.049	64.815	21.867	1.00	20.00
TER									
HETATM		Cl	INH3A	1	58.776	51.045	11.645	0.00	0.00
HETATM	2	N2	INH3A	1	58.172	52.218	11.841	0.00	0.00
HETATM	3	C3	INH3A	1	58.936	53.310	12.056	0.00	0.00
HETATM	4	C4	INH3A	1	60.320	53.244	12.077	0.00	0.00
HETATM	5	C5	INH3A	1	60.887	51.924	11.859	0.00	0.00
HETATM	6	N6	INH3A	1	60.101	50.854	11.646	0.00	0.00
HETATM	8	N8	INH3A	1	58.497	54.604	12.288	0.00	0.00
HETATM	9	C9	INH3A	1	59.673	55.293	12.446	0.00	0.00
HETATM	10	C10	INH3A	1	60.842	54.525	12.326	0.00	0.00
HETATM	12	N13	INH3A	1	62.289	51.734	11.876	0.00	0.00
HETATM	13	C14	INH3A	1	62.258	54.972	12.430	0.00	0.00
HETATM		C16	INH3A	1	57.098	55.079	12.339	0.00	0.00
HETATM	15	C17	INH3A	1	63.049	54.530	13.477	0.00	0.00
HETATM		C18	INH3A	1	64.374	54.941	13.612	0.00	0.00
HETATM		C19	INHSA	î	64.935	55.815	12.687	0.00	0.00
HETATM		C20	INHSA	1	64.131	56.249	11.643	0.00	0.00
HETATM		C21	INHSA	1	62.810	55.841	11.508	0.00	0.00
HETATM		N25	INH3A	1	66.225	56.236	12.788	0.00	0.00
HETATM		526	INH3A	1	66.995	56.113	14.217	0.00	0.00
HETATM		027		1	65.999	55.773	15.187	0.00	0.00
		021	TIME	2	05.399	53.773	40.207	0.00	0.00

 $\begin{array}{ll} \mbox{Docket/App No.:} & 2079.1037-001 \\ \mbox{Title: Method of Identifying Inhibitors of TIE-2} \\ \mbox{Inventors:} & \mbox{Nancy J. Bump $\it{et al.}$} \end{array}$

HETATM	26	028	INH3A	1	67.770	57.301	14.420	0.00	0.00
HETATM	27	C29	INH3A	1	68.100	54.741	14.032	0.00	0.00
HETATM	28	C30	INH3A	1	69.041	54.751	13.007	0.00	0.00
HETATM	29	C31	INH3A	1	69.873	53.654	12.825	0.00	0.00
HETATM	3.0	C32	INH3A	1	69.740	52.566	13.674	0.00	0.00
HETATM	31	C33	INH3A	1	68.801	52.539	14.696	0.00	0.00
HETATM	32	C34	INH3A	1	67.972	53.639	14.872	0.00	0.00
HETATM	37	F39	INH3A	1	70.540	51.507	13.502	0.00	0.00
HETATM	39	F41	INH3A	1	64.638	57.094	10.735	0.00	0.00
HETATM	40	C42	INH3A	1	56.781	55.784	13.669	0.00	0.00
HETATM	41	C43	INH3A	1	55.311	56.219	13.720	0.00	0.00
HETATM	42	C44	INH3A	1	54.962	57.130	12.528	0.00	0.00
HETATM	43	C45	INH3A	1	55.278	56.419	11.202	0.00	0.00
HETATM	44	C46	INH3A	1	56.748	55.981	11.144	0.00	0.00
HETATM	53	C55	INH3A	1	53.385	58.715	13.548	0.00	0.00
HETATM	54	C56	INH3A	1	51.998	59.356	13.419	0.00	0.00
HETATM	55	N57	AEHMI	1	50.930	58.353	13.520	0.00	0.00
HETATM	56	C58	INH3A	1	51.136	57.302	12.516	0.00	0.00
HETATM	57	C59	INH3A	1	52.522	56.662	12.658	0.00	0.00
HETATM	58	N60	INH3A	1	53.588	57.668	12.536	0.00	0.00
HETATM	68	C70	INH3A	1	49.599	58.958	13.416	0.00	0.00
TER									00

CRYST	86.	000	86	. 00	00 112.0	00 90.0	0 90.00	90.00	P42212
SCALE1		0.0	1163		0.00000	0.0000	0	0.00000	
SCALE2		0.00	0000		0.01163	0.0000	0	0.00000	
SCALE3		0.00	0000		0.00000	0.0089	3	0.00000	
ATOM	1	N	PRO	Α	817	8.606	38.803	6.968	1.00 63.06
ATOM	2	CA	PRO	Α	817	9.750	39.629	6.436	1.00 62.53
ATOM	3	C	PRO	A	817	10.180	38.953	5.133	1.00 62.97
ATOM	4	0	PRO	А	817	10.749	37.851	5.149	1.00 59.85
ATOM	5	CB	PRO	Α	817	10.807	39.752	7.499	1.00 62.45
ATOM	6	N	VAL	Α	818	9.794	39.542	3.998	1.00 63.22
ATOM	7	CA	VAL	Α	818	10.112	38.916	2.711	1.00 66.18
ATOM	8	С	VAL	Α	818	11,172	39.708	1.952	1.00 67.24
ATOM	9	0	VAL	Α	818	11.086	40.927	1.837	1.00 68.73
ATOM	10	CB	VAL	Α	818	8.866	38.691	1.843	1.00 66.96
ATOM	11	CG1	VAL	Α	818	9.133	37.632	0.770	1.00 67.29
ATOM	12	CG2	VAL	А	818	7.637	38.224	2.629	1.00 66.80
ATOM	13	N	LEU			12.192	39.014	1.464	1.00 67.40
ATOM	14	CA	LEU			13.300	39.569	0.705	1.00 67.89
ATOM	15	С	LEU			13.445	38.938	-0.680	1.00 68.53
ATOM	16	0	LEU		819	13.179	37.750	-0.875	1.00 67.98
ATOM	17	CB	LEU			14.589	39.374	1.493	1.00 67.17
ATOM	18	N	ASP			13.854	39.728	-1.668	1.00 70.32
ATOM	19	CA	ASP			13.962	39.181	-3.018	1.00 74.15
ATOM	20	C	ASP		820	15.382	38.826	-3.421	1.00 75.07
ATOM	21	ō	ASP			16.390	39.377	-2.978	1.00 74.87
ATOM	22	CB	ASP			13.314	40.147	-4.017	1.00 76.15
ATOM	23	CG	ASP			13.968	41.518	-4.054	1.00 78.23
ATOM	24	ODI	ASP		820	14.712	41.846	-3.092	1.00 79.04
ATOM	25	OD2	ASP			13.712	42.246	-5.051	1.00 78.55
ATOM	26	N	TRP			15.489	37.870	-4.336	1.00 77.12
ATOM	27	CA	TRP			16.794	37.480	-4.871	1.00 80.00
ATOM	2.8	C	TRP		821	17.288	38.671	-5.674	1.00 80.90
ATOM	29	ō	TRP			16.560	39.677	-5.750	1.00 82.56
ATOM	30	CB	TRP		821	16.640	36.237	-5.738	1.00 81.50
ATOM	31	CG	TRP		821	17.979	35.683	-6.126	1.00 84.29
ATOM	32	CD1	TRP			18.770	36.052	-7.174	1.00 85.04
ATOM	33	CD2	TRP		821	18.686	34.639	-5.443	1.00 85.54
ATOM	34	NE1	TRP		821	19.932	35.323	-7.184	1.00 85.91
ATOM	3.5	CE2	TRP		821	19.895	34.435	-6.138	1.00 86.16
ATOM	36	CE3			821	18.402	33.854	-4.317	1.00 85.72
ATOM	37	CZ2	TRP			20.822	33.474	-5.736	1.00 86.76
ATOM	3.8	CZ3	TRP			19.317	32.899	-3.914	1.00 86.12
ATOM	39	CH2	TRP			20.513	32.723	-4.632	1.00 86.81
ATOM	40	N	ASN			18.490	38.703	-6.220	1.00 80.99
ATOM	41	CA	ASN			18.941	39.868	-6.995	1.00 81.52
ATOM	42	C	ASN			18.729	41.071	-6.079	1.00 80.56
ATOM	43	ō			822	18.110	42.084	-6.381	1.00 81.67
ATOM	44	CB	ASN			18.164	39.937	-8.312	1.00 83.00
ATOM	45	CG			822	19.059	40.084	-9.532	1.00 84.08
ATOM	46	OD1				20.168	40.617	-9.420	1.00 84.25
ATOM	47	ND2	ASN			18.581		-10.679	1.00 84.49
ATOM	4.8	N	ASP			19.204	40.923	-4.856	1.00 78.69
ATOM	49	CA	ASP			19.120	41.815	-3.723	1.00 76.89
ATOM	50	c	ASP	A	823	19.874	41.123	-2.568	1.00 74.92
ATOM	51	0	ASP	A	823	19.952	41.542	-1.417	1.00 75.11
ATOM	52	CB	ASP		823	17.695	42.112	-3.299	1.00 77.66
ATOM	53	CG			823	17.306	43.572	-3.217	1.00 78.83
		~0	1101	-	020	1,.300	25.512	J.21/	1.00 /0.05

ATOM	54	OD1	ASP A	A 823	17.885	44.406	-3.955	1.00	79.53
ATOM	55	OD2	ASP A	823	16.391	43.945	-2.444		78.52
ATOM	56	N	ILE A		20.438	39.973	-2.919		71.67
ATOM	57	CA	ILE A		21.270	39.189	-2.030		69.30
ATOM	58	C	ILE A		22.624				
ATOM	59	ō	ILE A			39.046	-2.750		67.35
ATOM	60	CB	ILE A		22.678	38.352	-3.770		65.47
ATOM					20.744	37.783	-1.696		69.43
ATOM	61	CG1			19.356	37.733	-1.074	1.00	69.93
	62	CG2			21.752	37.046	-0.820	1.00	69.07
ATOM	63	CD1			19.156	38.009	0.386	1.00	71.48
MOTA	64	N	LYS P		23.649	39.735	-2.252	1.00	65.03
ATOM	65	CA	LYS A	825	24.977	39.581	-2.829	1.00	63.66
ATOM	66	C	LYS A	825	25.810	38.677	-1.903		62.88
ATOM	67	0	LYS A	825	26.290	39.103	-0.850		60.46
ATOM	68	CB	LYS A	825	25.688	40.893	-3.082		63.33
ATOM	69	N	PHE A	826	25.952	37.420	-2.315		62.22
ATOM	70	CA	PHE A		26.745	36.434	-1.595		
ATOM	71	C	PHE A		28.243	36.752			63.65
ATOM	72	0	PHE A				-1.654		64.85
ATOM	73	CB	PHE A		28.806	36.978	-2.738		65.98
ATOM	74				26.535	35.019	-2.151		63.23
		CG	PHE A		25.242	34.324	-1.828		63.28
ATOM	75	CD1	PHE A		24.194	34.262	-2.742	1.00	63.47
MOTA	76	CD2	PHE A		25.068	33.738	-0.587	1.00	62.78
ATOM	77	CE1	PHE A		23.013	33.606	-2.421	1.00	63.26
ATOM	78	CE2	PHE A	826	23.893	33.090	-0.261	1.00	63.76
ATOM	79	CZ	PHE A	826	22.859	33.026	-1.183		63.42
ATOM	80	N	GLN A	827	28.933	36.771	-0.514		64.73
ATOM	81	CA	GLN A	827	30.359	37.048	-0.474		63.67
ATOM	82	C	GLN A		31.182	35.763	-0.387		
ATOM	83	0	GLN A		31.703	35.217	-1.356		61.84
ATOM	84	CB	GLN A		30.736				
ATOM	85	CG	GLN A			37.884	0.748		65.45
ATOM	86	CD	GLN A		29.641	38.676	1.428		69.14
ATOM	87	OE1			29.805	40.166	1.185		71.09
ATOM			GLN A		29.364	40.617	0.124		72.36
ATOM	88	NE2	GLN A		30.442	40.865	2.124		71.89
	89	N	ASP A	828	31.371	35.286	0.838	1.00	61.57
ATOM	90	CA		828	32.237	34.122	1.034	1.00	62.37
ATOM	91	C	ASP A		31.576	33.071	1.883	1.00	61.37
ATOM	92	0	ASP A	828	30.330	32.899	1.910	1.00	63.34
ATOM	93	CB	ASP A	828	33.605	34.623	1.532	1.00	63.30
ATOM	94	CG	ASP A	828	33.536	35.073	2.977	1.00	65.22
ATOM	95	OD1	ASP A	828	34.629	35.346	3.505		66.32
ATOM	96	OD2	ASP A	828	32.418	35.135	3.513		67.27
ATOM	97	N	VAL A		32.332	32.174	2.503		59.16
ATOM	98	CA	VAL A		31.820	31.095	3.339		
ATOM	99	C		829	32.101	31.413			56.81
ATOM	100		VAL A				4.805	1.00	
ATOM	101		VAL A		33.252	31.767	5.119	1.00	
ATOM	102				32.462	29.753	2.948	1.00	
			VAL A		32.035	28.658	3.909	1.00	
ATOM	103		VAL A		32.111	29.383	1.513	1.00	
ATOM	104	N	ILE A		31.106	31.314	5.693	1.00	56.36
ATOM	105		ILE A		31.360	31.613	7.108	1.00	54.69
ATOM	106		ILE A		31.971	30.371	7.750	1.00	54.51
ATOM	107		ILE A	830	32.927	30.411	8.507	1.00	
ATOM	108	CB	ILE A	830	30.170	32.157	7.898		52.84
ATOM	109	CG1	ILE A	830	29.780	33.560	7.374		52.48
ATOM	110	CG2	ILE A	830	30.518	32.300	9.375	1.00	
					20.010	500	2.3.3	2.00	· 14

ATOM	111	CD1	ILE	'n	020	28.389	34.012	7.808	1.00 52.01
ATOM	112	N			831		29.232	7.808	1.00 54.93
ATOM	113	CA			831	31.431	27.959	7.866	1.00 54.93
ATOM	114	C			831	30.703		7.878	1.00 57.73
ATOM					831		27.066		
ATOM	115	O N			832	29.687	27.433	7.281	1.00 59.66
	116					30.811	25.963	8.594	1.00 62.36
ATOM	117	CA			832	29.649	25.080	8.634	1.00 65.54
ATOM	118	C			832	28.918	25.256	9.956	1.00 67.03
ATOM	119	0			832	29.525	25.480	10.982	1.00 65.58
MOTA	120	CB			832	30.079	23.647	8.389	1.00 65.24
ATOM	121	CG			832	29.979	22.748	9.615	1.00 64.68
ATOM	122	CD			832	30.771	21.493	9.247	1.00 65.38
ATOM	123	OE1			832	31.871	21.394	9.838	1.00 65.15
ATOM	124	OE2	GLU			30.232	20.771	8.386	1.00 64.01
ATOM	125	N	GLY			27.605	25.128	9.870	1.00 71.16
MOTA	126	CA	GLY	Α	833	26.741	25.268	11.048	1.00 75.85
ATOM	127	C	GLY	Α	833	25.973	23.945	11.138	1.00 79.10
ATOM	128	0	GLY	Α	833	26.489	22.959	11.666	1.00 80.05
ATOM	129	N	ASN	Α	834	24.750	23.982	10.627	1.00 80.77
ATOM	130	CA	ASN	Α	834	23.887	22.807	10.614	1.00 82.57
ATOM	131	C	ASN	А	834	23.055	22.917	9.332	1.00 82.72
ATOM	132	0	ASN			22.709	24.047	8.973	1.00 83.47
ATOM	133	CB	ASN			22.974	22.712	11.826	1.00 83.64
ATOM	134	CG	ASN			23.565	22.227	13.122	1.00 84.87
ATOM	135		ASN			23.040	22.476	14.214	1.00 85.57
ATOM	136	ND2	ASN			24.692	21.516	13.114	1.00 85.28
ATOM	137	N	PHE			22.813	21.799	8.663	1.00 82.37
ATOM	138	CA	PHE			22.018	21.747	7.436	1.00 81.44
ATOM	139	C	PHE			22.770	22.311	6.227	1.00 79.71
ATOM	140	0	PHE						
ATOM	141	CB	PHE			22.207	22.742	5.221	1.00 80.02
ATOM	142	N	GLY			20.656	22.423	7.609	1.00 81.62
ATOM							22.257	6.306	
ATOM	143 144	CA C	GLY			25.011	22.771	5.308	1.00 73.64
			GLY			25.714	24.008	5.875	1.00 70.61
ATOM	145	0	GLY			25.485	24.453	7.008	1.00 71.32
ATOM	146	N	GLN			26.589	24.607	5.081	1.00 67.00
ATOM	147	CA	GLN			27.288	25.779	5.584	1.00 64.94
ATOM	148	C	GLN			26.303	26.943	5.749	1.00 61.14
ATOM	149	0	GLN			25.079	26.947	5.627	1.00 62.09
ATOM	150	CB	GLN			28.510	26.214	4.782	1.00 65.56
ATOM	151	CG	GLN			28.323	26.175	3.277	1.00 68.22
ATOM	152	CD	GLN			28.499	24.771	2.717	1.00 70.10
ATOM	153	OE1	GLN			27.540	23.989	2.498	1.00 71.35
ATOM	154	NE2	GLN			29.776	24.447	2.508	1.00 69.74
ATOM	155	N	VAL			26.949	27.991	6.223	1.00 56.19
ATOM	156	CA	VAL	A	838	26.368	29.284	6.530	1.00 52.12
ATOM	157	C	VAL	А	838	27.166	30.196	5.612	1.00 51.49
ATOM	158	0	VAL			28.401	30.088	5.669	1.00 50.02
ATOM	159	CB	VAL	A	838	26.657	29.586	8.002	1.00 50.54
ATOM	160	CG1	VAL	A	838	26.258	30.989	8.386	1.00 48.67
MOTA	161	CG2	VAL	A	838	25.974	28.553	8.890	1.00 48.75
ATOM	162	N	LEU	Α	839	26.512	30.915	4.719	1.00 50.28
ATOM	163	CA	LEU	Α	839	27.308	31.782	3.831	1.00 48.12
ATOM	164	C	LEU	A	839	27.210	33.217	4.324	1.00 48.21
ATOM	165	0	LEU	Α	839	26.364	33.580	5.139	1.00 46.74
ATOM	166	CB	LEU	A	839	26.831	31.625	2.395	1.00 47.75
ATOM	167	CG	LEU			26.828	30.229	1.803	1.00 48.45
								1.000	

ATOM	168	CD1	LEU	2.	839	26.155	30.260	0.433	1.00 47.96
ATOM	169		LEU			28.160	29.519	1.717	1.00 44.56
ATOM	170	N	LYS			28.053	34.107	3.847	1.00 47.52
ATOM	171	CA			840	27.984	35.508	4.234	1.00 48.47
ATOM	172	C	LYS		840	27.434	36.369	3.109	1.00 49.26
ATOM	173	0	LYS		840	27.837	36.150	1.960	1.00 49.21
ATOM	174	CB			840	29.393	35.943	4.654	1.00 49.21
ATOM	175	CG			840	29.320	37.059	5.668	1.00 49.85
ATOM	176	CD	LYS		840	29.716			
ATOM	177	CE	LYS				38.398	5.125	1.00 49.60
ATOM	178	NZ	LYS			29.768	39.457	6.225	1.00 50.13
						31.184	39.749	6.580	1.00 51.35
ATOM	179	N	ALA			26.486	37.270	3.389	1.00 51.52
ATOM	180	CA	ALA			25.968	38.108	2.312	1.00 53.29
ATOM	181	С	ALA			25.768	39.564	2.726	1.00 54.51
ATOM	182	0	ALA			25.753	39.914	3.903	1.00 54.20
ATOM	183	CB	ALA			24.641	37.503	1.837	1.00 52.47
ATOM	184	N	ARG			25.564	40.398	1.714	1.00 57.16
ATOM	185	CA	ARG			25.154	41.784	1.915	1.00 60.23
ATOM	186	С	ARG			23.699	41.667	1.451	1.00 61.88
ATOM	187	0	ARG			23.499	41.023	0.416	1.00 63.40
ATOM	188	CB	ARG			25.900	42.835	1.119	1.00 61.09
ATOM	189	CG	ARG			27.301	43.137	1.622	1.00 62.77
MOTA	190	CD	ARG	Α	842	27.258	43.791	2.995	1.00 63.72
MOTA	191	NE	ARG	Α	842	26.985	45.231	2.928	1.00 64.65
ATOM	192	CZ	ARG	Α	842	26.963	45.986	4.017	1.00 65.52
ATOM	193	NH1	ARG	A	842	26.724	47.291	4.022	1.00 65.78
ATOM	194	NH2	ARG	A	842	27.158	45.436	5.214	1.00 66.80
ATOM	195	N	ILE	Α	843	22.745	42.047	2.281	1.00 63.86
ATOM	196	CA	ILE	A	843	21.322	41.935	1.983	1.00 66.38
ATOM	197	C	ILE	А	843	20.610	43.284	2.150	1.00 69.29
ATOM	198	0	ILE	Α	843	20.337	43.810	3.233	1.00 72.01
ATOM	199	CB	ILE	Α	843	20.524	40.846	2.715	1.00 64.76
ATOM	200	CG1	ILE	A	843	20.218	41.134	4.182	1.00 63.75
ATOM	201	CG2	ILE	Α	843	21.198	39.477	2.638	1.00 65.06
ATOM	202	CD1	ILE	А	843	19.030	40.372	4.733	1.00 61.60
ATOM	203	N	LYS	Α	844	20.274	43.844	0.975	1.00 70.72
ATOM	204	CA	LYS	Α	844	19.599	45.144	0.939	1.00 72.14
ATOM	205	C	LYS	Α	844	18.157	45.087	1.427	1.00 73.85
ATOM	206	0	LYS	Α	844	17.234	44.834	0.650	1.00 74.26
ATOM	207	CB	LYS	A	844	19.596	45.771	-0.449	1.00 71.35
ATOM	208	N	LYS	Α	845	17.931	45.392	2.697	1.00 75.42
ATOM	209	CA	LYS	Α	845	16.580	45.403	3.262	1.00 77.81
ATOM	210	C	LYS	Α	845	16.190	46.868	3.403	1.00 80.30
ATOM	211	0	LYS	Α	845	16.751	47.630	4.197	1.00 79.71
ATOM	212	CB	LYS		845	16.528	44.624	4.561	1.00 77.32
ATOM	213	CG	LYS	Α	845	15.188	44.450	5.231	1.00 76.89
ATOM	214	CD	LYS			15.318	43.734	6.572	1.00 76.27
ATOM	215	CE	LYS			13.956	43.469	7.205	1.00 75.52
ATOM	216	NZ	LYS			14.066	42.788	8.521	1.00 74.44
ATOM	217	N			846	15.243	47.333	2.610	1.00 82.92
ATOM	218	CA	ASP			14.674	48.627	2.374	1.00 84.85
ATOM	219	C			846	15.649	49.493	1.560	1.00 85.22
ATOM	220	ō	ASP			15.804	49.302	0.353	1.00 85.44
ATOM	221	CB	ASP	Ä	846	14.070	49.302	3.514	1.00 85.44
ATOM	222	CG			846	14.770	49.395	4.790	1.00 86.44
ATOM	223		ASP		846	15.058	50.942	5.029	1.00 88.52
ATOM	224	OD2	ASP			15.044	48.819	5.599	1.00 89.21
ALUM	224	ODZ	ASP	M	040	15.044	40.819	5.599	1.00 89.21

ATOM	225	N	GLY	70	047	16 227	F0 305	0 001		
ATOM	225	CA	GLY			16.337 17.317	50.395 51.266	2.231 1.590	1.00 8	
ATOM	225	C	GLY							
ATOM	228	0	GLY			18.593 19.555	51.154 51.871	2.430	1.00 8	
ATOM	229	N	LEU			18.493	50.239	3.396	1.00 8	
ATOM	230	CA	LEU			19.634	49.951	4.250	1.00	
ATOM	231	CA	LEU			20.311				
ATOM	232	0	LEU			19.608	48.732 47.760	3.617	1.00	
ATOM	232	CB	LEU			19.195	49.564	5.658	1.00	
ATOM	234	CG	LEU			18.312	50.582	6.388	1.00	
ATOM	235	CD1	LEU			17.346	49.858	7.312	1.00	
ATOM	236		LEU			19.184	51.563	7.157	1.00	
ATOM	237	N	ARG			21.592	48.863	3.326	1.00	
ATOM	238	CA	ARG			22.332	47.696	2.850	1.00	
ATOM	239	C	ARG			22.830	47.095	4.175	1.00	
ATOM	240	ō	ARG			23.153	47.922	5.036	1.00 6	
ATOM	241	CB	ARG			23.493	48.031	1.941	1.00	
ATOM	242	CG	ARG			23.308	47.798	0.452	1.00	
ATOM	243	CD	ARG			24.483	46.995	-0.110	1.00	
ATOM	244	NE	ARG			25.606	47.792	-0.586	1.00	
MOTA	245	CZ	ARG			26.848	47.399	-0.871	1.00	
ATOM	246	NH1	ARG			27.183	46.121	-0.715	1.00	
ATOM	247	NH2	ARG			27.739	48.290	-1.305	1.00	
MOTA	248	N	MET			22.777	45.781	4.369	1.00 6	
ATOM	249	CA			850	23.293	45.285	5.655	1.00	
ATOM	250	С	MET			23.898	43.883	5.493	1.00	
ATOM	251	0	MET			23.690	43.197	4.494	1.00 5	
ATOM	252	CB	MET	A	850	22.245	45.279	6.757	1.00 5	
ATOM	253	CG			850	21.296	44.096	6.631	1.00 5	
MOTA	254	SD	MET			19.724	44.280	7.443	1.00 5	
ATOM	255	CE	MET			20.128	44.922	9.049	1.00 5	
ATOM	256	N	ASP .	Α	851	24.651	43.563	6.548	1.00 5	
ATOM	257	CA	ASP .	A	851	25.299	42.268	6.600	1.00 4	
ATOM	258	С	ASP .	А	851	24.332	41.192	7.084	1.00 4	
MOTA	259	0	ASP .	A	851	23.630	41.457	8.086	1.00 4	2.14
ATOM	260	CB	ASP .	Α	851	26.379	42.285	7.697	1.00 5	50.01
ATOM	261	CG	ASP .	A	851	27.669	42.933	7.256	1.00 5	0.84
MOTA	262	OD1	ASP .	Α	851	28.043	42.801	6.057	1.00 5	1.87
MOTA	263	OD2	ASP .			28.272	43.563	8.144	1.00 5	0.81
MOTA	264	N	ALA .			24.472	39.961	6.632	1.00 4	15.45
ATOM	265	CA	ALA .			23.622	38.884	7.138	1.00 4	2.89
MOTA	266	C	ALA .			24.373	37.570	7.066	1.00 4	2.71
ATOM	267	0	ALA .			25.336	37.518	6.303	1.00 4	13.78
ATOM	268	CB	ALA .			22.397	38.727	6.261	1.00 4	1.61
ATOM	269	N	ALA .			23.847	36.577	7.785	1.00 4	13.18
MOTA	270	CA	ALA .			24.394	35.222	7.668	1.00 4	13.19
MOTA	271	C	ALA .			23.300	34.446	6.931	1.00 4	15.23
MOTA	272	0	ALA .			22.122	34.570	7.296	1.00 4	
MOTA	273	CB	ALA.			24.725	34.651	9.043	1.00 4	
ATOM	274	N	ILE .			23.599	33.717	5.863	1.00 4	
ATOM	275	CA	ILE .			22.561	33.051	5.093	1.00 4	
ATOM	276	С	ILE .			22.583	31.537	5.228	1.00 5	
ATOM	277	0	ILE .			23.643	30.913	5.101	1.00 5	
MOTA	278	CB	ILE .			22.686	33.334	3.581	1.00 4	
ATOM	279	CG1	ILE .			22.754	34.819	3.268	1.00 4	
MOTA	280	CG2	ILE .			21.553	32.685	2.794	1.00 4	
MOTA	281	CD1	ILE .	Α	854	21.509	35.654	3.433	1.00 4	15.48

COCKER TOUGH

ATOM	282	N	LYS A	855	21.408	30.949	5.453	1.00 51.72
ATOM	283	CA	LYS A		21.355	29.474	5.425	1.00 54.33
ATOM	284	C	LYS A		20.240	29.052	4.458	1.00 55.89
ATOM	285	ō	LYS A		19.276	29.786	4.205	1.00 52.41
ATOM	286	CB		855	21.271	28.892	6.808	1.00 55.64
ATOM	287	CG	LYS A		19.914	28.834	7.487	1.00 58.25
ATOM	288	CD		855	20.052	28.092		1.00 59.55
ATOM	289	CE	LYS A				8.807	
ATOM		NZ			18.987	27.027	9.025	1.00 60.12
	290				19.484	26.165	10.151	1.00 60.89
ATOM ATOM	291 292	N CA	ARG A		20.386	27.871	3.871	1.00 59.82
					19.419	27.341	2.915	1.00 63.71
ATOM	293	C	ARG A		18.809	26.009	3.309	1.00 66.24
ATOM	294	0	ARG A		19.456	25.004	3.565	1.00 66.29
ATOM	295	CB	ARG A		20.126	27.258	1.555	1.00 63.38
ATOM	296	N		857	17.486	25.951	3.418	1.00 69.77
ATOM	297	CA		857	16.718	24.748	3.728	1.00 73.04
ATOM	298	C		857	15.960	24.381	2.447	1.00 75.83
ATOM	299	0		857	16.149	25.126	1.472	1.00 77.44
ATOM	300	CB		857	15.761	24.965	4.887	1.00 72.49
ATOM	301	N		858	15.174	23.321	2.404	1.00 78.15
ATOM	302	CA	LYS A		14.449	22.985	1.184	1.00 80.35
ATOM	303	C	LYS A		13.181	22.168	1.417	1.00 81.76
ATOM	304	0	LYS A		13.118	21.298	2.282	1.00 82.29
ATOM	305	CB	LYS A		15.320	22.196	0.212	1.00 80.34
ATOM	306	N	GLU A		12.171	22.427	0.593	1.00 82.86
ATOM	307	CA	GLU A		10.905	21.705	0.631	1.00 83.98
ATOM	308	C	GLU A		10.372	21.378	2.024	1.00 84.84
MOTA	309	0	GLU A		9.465	20.540	2.160	1.00 85.54
ATOM	310	CB	GLU A	859	11.040	20.388	-0.143	1.00 83.34
TER								
ATOM	311	N		868	3.887	24.257	9.102	1.00 74.33
ATOM	312	CA	ASP B		4.969	23.506	9.742	1.00 73.45
ATOM	313	С	ASP B		6.151	24.465	9.894	1.00 72.92
ATOM	314	0	ASP B		6.215	25.236	10.848	1.00 72.75
ATOM	315	CB		868	5.345	22.276	8.927	1.00 73.09
ATOM	316	N	PHE B		6.973	24.491	8.845	1.00 71.93
ATOM	317	CA `	PHE B		8.128	25.356	8.739	1.00 71.39
ATOM	318	С	PHE B		7.722	26.812	8.514	1.00 69.85
ATOM	319	0		869	8.507	27.721	8.789	1.00 68.53
ATOM	320	CB	PHE B		9.086	24.894	7.635	1.00 72.16
ATOM	321	N	ALA B		6.485	27.041	8.084	1.00 68.66
ATOM	322	CA	ALA B		6.008	28.412	7.917	1.00 67.79
ATOM	323	C	ALA B		5.699	28.972	9.300	1.00 66.69
ATOM	324	0	ALA B		5.914	30.142	9.612	1.00 67.76
ATOM	325	CB	ALA B		4.786	28.421	7.009	1.00 67.73
ATOM	326	N	GLY B		5.125	28.124	10.156	1.00 64.74
ATOM	327	CA	GLY B		4.746	28.539	11.506	1.00 63.48
ATOM	328	C	GLY B		5.968	28.696	12.407	1.00 63.38
ATOM	329	0	GLY B		6.078	29.586	13.241	1.00 62.27
ATOM ATOM	330	N CA		872	6.936	27.789	12.259	1.00 63.08
	331		GLU B		8.163	27.830	13.033	1.00 62.41
ATOM ATOM	332 333	0	GLU B		8.870	29.166	12.865	1.00 59.48
ATOM	334	CB	GLU B		9.299	29.759	13.849	1.00 59.18
ATOM	335	CG	GLU B		9.104	26.684	12.627	1.00 64.92
ATOM	335	CD	GLU B		8.756 9.191	25.334	13.218	1.00 67.28
ATOM	337		GLU B		8.848		12.4/4	1.00 68.33
111-011	227	ULL	Juo B	0/2	8.648	22.953	12.910	1.00 09.51

ATOM	338	OE2	GLU	B 872	9.882	24.117	11.435	1.00	69.53
ATOM	339	N	LEU :	B 873	9.004	29.664	11.648	1.00	
ATOM	340	CA	LEU :	873	9.635	30.916	11.312		55.15
ATOM	341	C	LEU :	B 873	8.988	32.099	12.034	1.00	
ATOM	342	0	LEU :	873	9.656	33.045	12.483		53.19
ATOM	343	CB	LEU :	873	9.629	31.206	9.816	1.00	
ATOM	344	CG	LEU :	873	10.436	30.326	8.876		56.52
ATOM	345	CD1	LEU I	873	10.416	30.920	7.466		56.98
ATOM	346	CD2	LEU I	873	11.886	30.139	9.305		57.06
ATOM	347	N	GLU 1	874	7.663	32.055	12.083		53.38
ATOM	348	CA	GLU 1		6.839	33.058	12.743	1.00	53.73
ATOM	349	C	GLU 1		7.208	33.198	14.215	1.00	50.89
ATOM	350	0	GLU :		7.431	34.279	14.773	1.00	48.19
ATOM	351	CB	GLU I		5.379	32.579	12.639	1.00	57.54
ATOM	352	CG	GLU H		4.388	33.300	13.533	1.00	61.33
ATOM	353	CD	GLU I	874	3.007	32.638	13.433	1.00	64.62
MOTA	354		GLU I		2.075	33.216	14.045	1.00	66.21
ATOM	355	OE2	GLU E	874	2.876	31.577	12.771	1.00	64.60
ATOM	356	N	VAL E	875	7.278	32.004	14.839	1.00	48.16
ATOM	357	CA	VAL E		7.665	31.965	16.266		47.64
ATOM	358	C	VAL E		9.051	32.599	16.426	1.00	46.85
ATOM	359	0	VAL E	875	9.211	33.498	17.257	1.00	45.14
ATOM	360	CB	VAL E		7.523	30.545	16.799		47.78
ATOM	361	CG1	VAL E		8.477	30.264	17.946		48.21
ATOM	362	CG2	VAL E		6.077	30.272	17.240	1.00	47.41
ATOM	363	N	LEU E		10.000	32.278	15.538	1.00	47.87
ATOM	364	CA	LEU E		11.348	32.838	15.552	1.00	50.02
ATOM	365	C	LEU E		11.435	34.322	15.245	1.00	50.20
ATOM	366	0	LEU E		12.285	34.988	15.845	1.00	51.04
ATOM	367	CB	LEU E		12.308	32.074	14.611	1.00	48.16
ATOM	368	CG	LEU E		12.598	30.663	15.159	1.00	49.64
ATOM	369	CD1	LEU B		13.303	29.816	14.116	1.00	48.69
ATOM	370	CD2	LEU B		13.407	30.766	16.452	1.00	51.42
ATOM	371	N	CYS B		10.607	34.849	14.358	1.00	50.72
ATOM ATOM	372	CA	CYS B		10.638	36.276	14.029	1.00	51.41
ATOM	373	C	CYS B		10.130	37.090	15.215	1.00	50.29
ATOM	374	0	CYS B		10.630	38.171	15.550	1.00	49.69
ATOM	375	CB	CYS B		9.777	36.555	12.788	1.00	53.49
ATOM	376 377	SG	CYS B		9.320	38.304	12.668	1.00	56.75
ATOM		N	LYS B		9.155	36.480	15.922		49.77
ATOM	378 379	CA C	LYS B		8.602	37.082	17.122		49.11
ATOM	380	0			9.567	37.033	18.298		47.30
ATOM			LYS B		9.418	37.925	19.128		47.68
ATOM	381 382	CB CG	LYS B	878	7.284	36.415	17.561	1.00	51.27
ATOM	383	CD	LYS B	878 878	6.097	36.821	16.728	1.00	53.14
ATOM	384	CE	LYS B	878	5.072	35.740	16.473	1.00	55.56
ATOM	385	NZ	LYS B	878	4.132	35.453	17.638		55.88
ATOM	386	N	LEU B	879	3.445	34.138	17.433		57.41
ATOM	387	CA	LEU B	879	10.495	36.091	18.403		44.23
ATOM	388	C	LEU B		11.388	36.049	19.550	1.00	
ATOM	389	0	LEU B	879 879	12.665	36.881	19.317	1.00	
ATOM	390	CB	LEU B	879	13.291 11.857	37.300	20.264		39.35
ATOM	391	CG	LEU B	879		34.606	19.819		41.39
ATOM	392		LEU B	879	10.790	33.580	20.246		40.34
ATOM	393		LEU B	879	11.327 10.378	32.180	20.076		40.43
ATOM	394	N	GLY B		12.974	33.826 37.194	21.693	1.00	
	_	-	2		12.5/4	37.194	18.075	1.00	40.80

Docket/App No.: 2079.1037-001

Title: Method of Identifying Inhibitors of TIE-2 Inventors: Nancy J. Bump etal.

ATOM	395	CA	GLY	-	202	14.164	25 252	17.686	1.00 42.66
ATOM	395	C			880	14.164	37.870 39.226	18.185	1.00 42.66
ATOM	395	0	GLY	В	880	15.698	39.526	18.103	1.00 46.29
ATOM	398	N	HIS	В	881	13.580	40.053	18.637	1.00 40.29
ATOM	399	CA	HIS	В	881	13.759	41.403	19.105	1.00 42.86
ATOM	400	CA	HIS	В	881	14.619	41.403	20.370	1.00 43.65
ATOM	400	0	HIS	В	881	15.539	42.203	20.370	1.00 39.48
ATOM	402	CB	HIS	В	881				1.00 43.05
ATOM	402	CG	HIS	В	881	12.417 11.628	42.127	19.236	1.00 47.39
ATOM	403		HIS	В	881				
ATOM	404		HIS		881	10.412	41.442	20.685	1.00 53.62
ATOM	405		HIS		881		42.576	21.711	
ATOM	405	NE2	HIS		881	10.057	41.591	21.975	1.00 55.27
						10.966	42.286	22.647	1.00 55.05
ATOM	408	N	HIS		882	14.422	40.401	21.250	1.00 35.00
ATOM	409	CA	HIS		882	15.234	40.280	22.473	1.00 33.75
ATOM	410	C	HIS		882	16.695	40.394	22.053	1.00 29.63
ATOM	411	0	HIS		882	17.099	39.702	21.115	1.00 32.51
ATOM	412	CB	HIS		882	14.977	38.947	23.240	1.00 29.31
ATOM	413	CG	HIS		882	15.458	39.007	24.665	1.00 28.91
ATOM	414		HIS	В	882	16.739	38.861	25.208	1.00 28.25
ATOM	415		HIS	В	882	14.687	39.334	25.705	1.00 27.99
ATOM	416		HIS		882	16.623	39.049	26.523	1.00 28.98
ATOM	417		HIS		882	15.346	39.333	26.866	1.00 26.63
ATOM	418	N	PRO		883	17.468	41.252	22.659	1.00 31.32
ATOM	419	CA	PRO		883	18.882	41.398	22.375	1.00 31.40
MOTA	420	C	PRO		883	19.687	40.158	22.658	1.00 32.62
ATOM	421	0	PRO		883	20.700	39.965	21.941	1.00 36.70
MOTA	422	CB	PRO		883	19.206	42.672	23.123	1.00 30.55
ATOM	423	CG	PRO		883	18.433	42.543	24.437	1.00 33.27
ATOM	424	CD	PRO		883	17.096	42.064	23.858	1.00 31.21
ATOM	425	N	ASN			19.290	39.189	23.448	1.00 33.73
ATOM	426	CA	ASN		884	19.999	37.942	23.685	1.00 32.47
ATOM	427	C	ASN	В	884	19.496	36.811	22.823	1.00 34.37
ATOM	428	0	ASN	В	884	19.901	35.659	23.051	1.00 34.65
MOTA	429	CB	ASN	В	884	19.952	37.596	25.173	1.00 33.46
MOTA	430	CG	ASN	В	884	20.404	38.649	26.117	1.00 36.23
ATOM	431		ASN	В	884	20.011	39.181	27.122	1.00 37.73
MOTA.	432	ND2	ASN	В	884	21.749	38.992	25.840	1.00 32.70
ATOM	433	N			885	18.623	37.014	21.825	1.00 32.48
ATOM	434	CA			885	18.185	36.032	20.859	1.00 34.12
ATOM	435	С	ILE	В	885	18.587	36.426	19.455	1.00 32.76
ATOM	436	0	ILE	В	885	18.359	37.539	18.982	1.00 33.37
ATOM	437	CB	ILE		885	16.662	35.743	21.004	1.00 33.83
ATOM	438	CG1			885	16.442	35.119	22.402	1.00 35.22
ATOM	439	CG2	ILE	В	885	16.088	34.847	19.922	1.00 33.58
ATOM	440	CD1	ILE	В	885	14.970	34.840	22.653	1.00 38.35
ATOM	441	N	ILE	В	886	19.261	35.557	18.697	1.00 34.99
ATOM	442	CA	ILE	В	886	19.694	35.965	17.333	1.00 37.58
ATOM	443	C	ILE	В	886	18.478	36.272	16.468	1.00 39.01
ATOM	444	0	ILE	В	886	17.526	35.459	16.453	1.00 38.20
ATOM	445	CB	ILE	В	886	20.693	34.967	16.752	1.00 38.15
ATOM	446	CG1	ILE	В	886	21.549	35.590	15.622	1.00 40.28
ATOM	447	CG2	ILE	В	886	19.985	33.776	16.206	1.00 38.96
ATOM	448	CD1	ILE	В	886	22.675	36.445	16.190	1.00 39.25
ATOM	449	N	ASN	В	887	18.472	37.380	15.731	1.00 38.67
ATOM	450	CA	ASN	В	887	17.268	37.824	15.016	1.00 40.23
ATOM	451	C	ASN	В	887	17.116	37.485	13.560	1.00 40.18

1 mov	452	0	ASN B	007	18.061	37.480	12.780	1.00 41.35
ATOM	453	CB	ASN B		17.153	39.347	15.231	1.00 40.41
ATOM ATOM	454	CG		887	15.888	39.999	14.697	1.00 40.25
ATOM	455	OD1		887	15.961	41.166	14.290	1.00 39.53
ATOM	456	ND2		887	14.746	39.340	14.692	1.00 38.70
ATOM	457	N		888	15.891	37.146	13.147	1.00 42.05
ATOM	458	CA	LEU B	888	15.624	36.781	11.744	1.00 43.89
ATOM	459	C		888	15.501	38.053	10.900	1.00 44.52
ATOM	460	0	LEU B	888	14.790	38.957	11.351	1.00 42.69
ATOM	461	CB	LEU B	888	14.321	35.988	11.680	1.00 45.35
ATOM	462	CG	LEU B	888	13.675	35.835	10.310	1.00 46.44
ATOM	463	CD1	LEU B	888	14.617	35.185	9.322	1.00 47.08
ATOM	464	CD2	LEU B	888	12.393	35.011	10.433	1.00 48.74
ATOM	465	N	LEU B	889	16.221	38.160	9.785	1.00 46.33
ATOM	466	CA		889	16.106	39.377	9.004	1.00 48.96
ATOM	467	C		889	15.178	39.162	7.822	1.00 48.91
ATOM	468	0		889	14.331	40.055	7.642	1.00 52.61
ATOM	469	CB		889	17.407	40.091	8.621	1.00 52.03
ATOM	470	CG		889	18.022	40.806	9.850	1.00 54.44
ATOM	471	CD1		889	18.709	39.713	10.624 9.535	1.00 56.62 1.00 56.92
ATOM	472	CD2		889	19.053 15.192	41.862 38.056	7.122	1.00 48.86
ATOM	473	N		890	14.281	37.806	6.027	1.00 49.19
ATOM	474	CA		890 890	14.348	36.393	5.478	1.00 51.62
ATOM	475	C		890	15.216	35.581	5.811	1.00 49.54
ATOM ATOM	476 477	N		891	13.367	36.080	4.619	1.00 52.67
ATOM	478	CA		891	13.339	34.779	3.956	1.00 55.84
ATOM	479	C	ALA B	891	13.195	35.036	2.454	1.00 58.68
ATOM	480	ō	ALA B	891	12.782	36.128	2.056	1.00 60.04
ATOM	481	CB		891	12.292	33.826	4.471	1.00 54.13
ATOM	482	N	CYS B	892	13.681	34.109	1.646	1.00 61.71
ATOM	483	CA	CYS B	892	13.618	34.248	0.200	1.00 64.65
ATOM	484	C	CYS B	892	13.505	32.847	-0.403	1.00 67.70
ATOM	485	0		892	14.279	31.955	-0.046	1.00 68.56
MOTA	486	CB	CYS B	892	14.817	34.942	-0.412	1.00 63.99 1.00 64.16
ATOM	487	SG	CYS B	892	14.859	34.973	-2.216	1.00 64.16 1.00 70.26
MOTA	488	N	GLU B	893	12.506	32.682	-1.262 -1.965	1.00 70.28
ATOM	489	CA	GLU B	893	12.337	31.411	-3.354	1.00 72.47
ATOM	490	C	GLU B	893 893	12.959 12.603	32.421	-4.134	1.00 72.44
ATOM ATOM	491 492	O CB		893	10.873	30.991	-2.027	1.00 74.16
ATOM	492	CG	GLU B	893	10.291	30.437	-0.736	1.00 76.17
ATOM	494	CD	GLU B	893	8.789	30.210	-0.801	1.00 77.74
ATOM	495	OE1		893	8.126	30.906	-1.611	1.00 78.37
ATOM	496	OE2		893	8.230	29.357	-0.069	1.00 78.86
ATOM	497	N	HIS B	894	13.922	30.697	-3.677	1.00 73.54
ATOM	498	CA	HIS B	894	14.594	30.700	-4.977	1.00 74.67
ATOM	499	C	HIS B	894	14.847	29.255	-5.401	1.00 74.91
ATOM	500	0	HIS B	894	15.025	28.386	-4.542	1.00 74.35
ATOM	501	CB	HIS B	894	15.857	31.531	-4.919	1.00 75.48
ATOM	502	CG	HIS B	894	16.558	31.697	-6.225	1.00 76.90
ATOM	503		HIS B	894	17.369	30.719	-6.752	1.00 77.63
MOTA	504		HIS B	894	16.587	32.733	-7.097	1.00 77.64
ATOM	505	CE1		894	17.880	31.150	-7.893	1.00 78.14
ATOM	506		HIS B		17.433	32.377	-8.119	1.00 77.87
ATOM	507	N	ARG B		14.774	28.959	-6.699 -7.214	1.00 74.84
ATOM	508	CA	ARG B	895	14.865	27.593	-/.214	2.00 /3.90

ATOM	509	C	ARG I	895	14.001	26.742	-6.281	1.00 74.16
ATOM	510	0	ARG I	895	12.911	27.249	-5.967	1.00 74.67
ATOM	511	CB	ARG I	895	16.262	27.053	-7.367	1.00 74.14
ATOM	512	N	GLY I	896	14.429	25.597	-5.769	1.00 73.62
ATOM	513	CA	GLY E	896	13.554	24.843	-4.878	1.00 74.58
ATOM	514	C	GLY I	896	13.801	24.946	~3.383	1.00 75.31
ATOM	515	0	GLY I	896	13.362	24.085	-2.599	1.00 74.62
ATOM	516	N	TYR I	897	14.568	25.958	-2.952	1.00 75.55
ATOM	517	CA	TYR I	897	14.937	26.107	-1.551	1.00 75.78
ATOM	518	C	TYR I	897	14.498	27.408	-0.882	1.00 73.41
ATOM	519	0	TYR I	897	14.296	28.420	-1.548	1.00 73.50
ATOM	520	CB	TYR I	897	16.466	26.038	-1.444	1.00 78.25
ATOM	521	CG	TYR I	897	17.225	24.811	-1.836	1.00 80.53
ATOM	522	CD1	TYR I	897	17.259	24.356	-3.145	1.00 81.37
ATOM	523	CD2	TYR I	897	17.982	24.114	-0.898	1.00 81.11
ATOM	524	CE1	TYR I	897	17.983	23.232	-3.498	1.00 82.95
ATOM	525	CE2	TYR I	897	18.712	22.994	-1.247	1.00 82.00
ATOM	526	CZ	TYR I	897	18.723	22.542	-2.554	1.00 82.42
ATOM	527	N	LEU E	898	14.434	27.417	0.450	1.00 70.37
ATOM	528	CA	LEU I	898	14.132	28.667	1.172	1.00 68.25
ATOM	529	C	LEU I	898	15.407	29.218	1.794	1.00 66.94
ATOM	530	0	LEU I	898	16.271	28.530	2.340	1.00 67.22
ATOM	531	CB	LEU I	898	12.957	28.443	2.089	1.00 67.63
ATOM	532	CG	LEU E	898	12.979	28.839	3.549	1.00 66.92
ATOM	533	CD1	LEU E	898	11.612	29.212	4.063	1.00 67.30
ATOM	534	CD2	LEU I	898	13.492	27.667	4.393	1.00 67.72
ATOM	535	N	TYR I	899	15.648	30.512	1.585	1.00 65.23
ATOM	536	CA	TYR I	899	16.871	31.191	2.019	1.00 61.95
ATOM	537	C	TYR I	899	16.601	32.001	3.262	1.00 60.81
ATOM	538	0	TYR I	899	15.646	32.797	3.247	1.00 61.40
ATOM	539	CB	TYR I	899	17.291	31.923	0.733	1.00 62.33
ATOM	540	CG	TYR I	899	17.999	31.028	-0.267	1.00 63.29
ATOM	541	CD1	TYR I	899	17.347	30.060	-1.018	1.00 63.92
ATOM	542	CD2	TYR I	899	19.373	31.154	-0.439	1.00 63.86
ATOM				899	18.025	29.235	-1.897	1.00 64.75
	543	CE1	TYR I		20.078			1.00 04.75
ATOM	544	CE1	TYR I		20.070	30.345	-1.317	1.00 64.75
ATOM ATOM				899	19.395	30.345	-1.317 -2.041	
	544	CE2	TYR I	899 899				1.00 64.65
ATOM	544 545	CE2 CZ	TYR I	899 899 899 899	19.395	29.384	-2.041 -2.918 4.397	1.00 64.65 1.00 65.94 1.00 66.41 1.00 56.58
ATOM ATOM	544 545 546	CE2 CZ OH	TYR I	899 899 899 899 900	19.3 9 5 20.089	29.384 28.577	-2.041 -2.918 4.397 5.625	1.00 64.65 1.00 65.94 1.00 66.41 1.00 56.58 1.00 52.46
ATOM ATOM ATOM	544 545 546 547	CE2 CZ OH N	TYR I	899 899 899 899 900	19.395 20.089 17.269	29.384 28.577 31.750	-2.041 -2.918 4.397	1.00 64.65 1.00 65.94 1.00 66.41 1.00 56.58
ATOM ATOM ATOM ATOM	544 545 546 547 548	CE2 CZ OH N CA	TYR I	8 899 8 899 8 899 8 900 8 900 8 900	19.395 20.089 17.269 17.006	29.384 28.577 31.750 32.506	-2.041 -2.918 4.397 5.625	1.00 64.65 1.00 65.94 1.00 66.41 1.00 56.58 1.00 52.46
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	544 545 546 547 548 549 550 551	CE2 CZ OH N CA C O CB	TYR 1 TYR 1 TYR 1 LEU 1 LEU 1 LEU 1 LEU 1	8 8 9 9 8 9 9 8 9 9 9 9 9 9 9 9 9 9 9 9	19.395 20.089 17.269 17.006 18.209 19.359 16.742	29.384 28.577 31.750 32.506 33.421 33.002 31.664	-2.041 -2.918 4.397 5.625 5.892 5.834 6.859	1.00 64.65 1.00 65.94 1.00 66.41 1.00 56.58 1.00 52.46 1.00 50.69 1.00 49.63 1.00 52.94
ATOM ATOM ATOM ATOM ATOM ATOM	544 545 546 547 548 549 551 552	CE2 CZ OH N CA C	TYR 1 TYR 1 TYR 1 LEU 1 LEU 1 LEU 1 LEU 1 LEU 1	8 8 9 9 8 9 9 8 9 9 0 0 8 9 0 0 8 9 0 0 8 9 0 0 8 9 0 0 8 9 0 0 8 9 0 0 0 8 9 0 0 0 8 9 0 0 0 8 9 0 0 0 8 9 0 0 0 0	19.395 20.089 17.269 17.006 18.209 19.359	29.384 28.577 31.750 32.506 33.421 33.002	-2.041 -2.918 4.397 5.625 5.892 5.834 6.859 6.845	1.00 64.65 1.00 65.94 1.00 66.41 1.00 56.58 1.00 52.46 1.00 50.69 1.00 49.63 1.00 52.94 1.00 53.46
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	544 545 546 547 548 549 550 551	CE2 CZ OH N CA C O CB CG CD1	TYR I	8 899 8 899 8 899 8 900 8 900 8 900 8 900 8 900 8 900	19.395 20.089 17.269 17.006 18.209 19.359 16.742	29.384 28.577 31.750 32.506 33.421 33.002 31.664	-2.041 -2.918 4.397 5.625 5.892 5.834 6.859	1.00 64.65 1.00 65.94 1.00 66.58 1.00 56.58 1.00 50.69 1.00 49.63 1.00 52.94 1.00 53.46
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	544 545 546 547 548 549 555 555 553 554	CE2 CZ OH N CA C O CB CG CD1	TYR 1 TYR 1 LEU 1	8 8 9 9 8 8 9 9 8 8 9 9 0 0 8 9 0 0 0 8 9 0 0 0 8 9 0 0 0 8 9 0 0 0 8 9 0 0 0 8 9 0 0 0 0	19.395 20.089 17.269 17.006 18.209 19.359 16.742 15.786 16.449	29.384 28.577 31.750 32.506 33.421 33.002 31.664 30.472 29.204 30.153	-2.041 -2.918 4.397 5.625 5.892 5.834 6.859 6.845 6.312 8.224	1.00 64.65 1.00 65.46 1.00 56.58 1.00 52.46 1.00 50.69 1.00 52.94 1.00 53.46 1.00 53.76
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	544 545 546 547 548 549 550 551 552 553	CE2 CZ OH N CA C O CB CG CD1 CD2 N	TYR 1 TYR 1 TYR 1 LEU 1	8 899 8 899 8 899 8 900 8 900 8 900 8 900 8 900 8 900 8 900 8 900	19.395 20.089 17.269 17.006 18.209 19.359 16.742 15.786 16.449 15.211 17.923	29.384 28.577 31.750 32.506 33.421 33.002 31.664 30.472 29.204 30.153 34.696	-2.041 -2.918 4.397 5.625 5.892 5.834 6.859 6.845 6.312 8.224 6.093	1.00 64.65 1.00 65.94 1.00 66.41 1.00 56.58 1.00 52.46 1.00 50.63 1.00 52.94 1.00 53.46 1.00 53.46 1.00 53.76 1.00 48.07
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	544 545 546 547 548 550 551 552 553 554 555 556	CE2 CZ OH N CA C O CB CG CD1 CD2 N	TYR 1 TYR 1 TYR 1 LEU 1 ALA 1	8 899 8 899 8 899 8 900 8 900 8 900 8 900 8 900 8 901 8 901	19.395 20.089 17.269 17.006 18.209 19.359 16.742 15.786 16.449 15.211 17.923 18.972	29.384 28.577 31.750 32.506 33.421 33.002 31.664 30.472 29.204 30.153 34.696 35.699	-2.041 -2.918 4.397 5.625 5.892 5.834 6.859 6.845 6.312 8.224 6.093 6.337	1.00 64.65 1.00 65.41 1.00 56.58 1.00 52.46 1.00 50.69 1.00 52.94 1.00 52.94 1.00 53.46 1.00 53.46 1.00 53.46 1.00 53.46 1.00 48.07 1.00 44.87
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	544 545 546 547 548 550 551 552 553 554 555 556 557	CE2 CZ OH N CA C O CB CG CD1 CD2 N CA C	TYR 1 TYR 1 LEU 1 ALA 1 ALA 1	8 899 8 899 8 899 8 900 8 900 8 900 8 900 8 900 8 900 8 901 8 901 8 901	19.395 20.089 17.269 17.006 18.209 19.359 16.742 15.786 16.449 15.211 17.923 18.972 18.893	29.384 28.577 31.750 32.506 33.421 33.002 31.664 30.472 29.204 30.153 34.696 35.699 36.119	-2.041 -2.918 4.397 5.625 5.892 5.834 6.859 6.845 6.312 8.224 6.093 6.337 7.800	1.00 64.65 1.00 65.94 1.00 66.41 1.00 56.58 1.00 52.46 1.00 49.69 1.00 49.69 1.00 53.46 1.00 53.76 1.00 48.07 1.00 44.87 1.00 44.87
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	544 545 546 547 548 550 551 555 555 555 556 557 558	CE2 CZ OH N CA C O CB CG CD1 CD2 N CA C	TYR 1 TYR 1 LEU 1 ALA 1 ALA 1 ALA 1	8 899 8 899 8 899 8 900 8 900 8 900 8 900 8 900 8 901 8 901 8 901 8 901	19.395 20.089 17.269 17.006 18.209 19.359 16.742 15.786 16.449 15.211 17.923 18.972 18.895	29.384 28.577 31.750 32.506 33.421 33.002 31.664 30.472 29.204 30.153 34.696 35.699 36.119 36.689	-2.041 -2.918 4.397 5.625 5.892 5.834 6.859 6.312 8.224 6.093 6.337 7.800 8.253	1.00 64.65 1.00 65.94 1.00 66.41 1.00 56.58 1.00 52.46 1.00 50.69 1.00 52.94 1.00 53.02 1.00 53.02 1.00 53.76 1.00 48.07 1.00 44.87 1.00 42.43
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	544 545 546 547 548 550 551 555 555 555 557 558 9	CE2 CZ OH N CA C O CB CG CD1 CD2 N CA C O CB CCA C C O CB	TYR 1 TYR 1 LEU 1 ALA 1 ALA 1 ALA 1	8 899 8 899 8 899 8 900 8 900 8 900 8 900 8 900 8 900 8 901 8 901 8 901 8 901 8 901	19.395 20.089 17.269 17.006 18.209 19.359 16.742 15.786 16.449 15.211 17.923 18.893 17.895 18.777	29.384 28.577 31.750 32.506 33.002 31.664 30.472 29.204 30.153 34.696 35.699 36.689 36.899	-2.041 -2.918 4.397 5.625 5.892 5.834 6.859 6.312 8.224 6.093 6.337 7.800 8.253 5.429	1.00 64.65 1.00 65.94 1.00 56.58 1.00 56.58 1.00 52.46 1.00 50.69 1.00 52.94 1.00 53.46 1.00 53.46 1.00 53.46 1.00 53.40 1.00 53.40 1.00 53.41 1.00 42.43 1.00 42.43 1.00 41.24
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	544 545 546 547 548 555 555 555 555 555 555 555 555 555	CE2 CZ OH N CA C O CB CG CD1 CD2 N CA C O CB N	TYR 1 TYR 1 LEU 1 ALA 1 ALA 1 ALA 1 ALA 1	8 8 9 9 8 8 9 9 8 8 9 9 9 0 0 8 9 9 0 0 0 8 9 9 0 0 0 8 9 0 0 0 8 9 0 0 1 8 9	19.395 20.089 17.269 17.006 18.209 19.359 16.742 15.786 16.449 15.211 17.923 18.972 18.893 17.895 18.777	29.384 28.577 31.750 32.506 33.421 33.002 31.664 30.472 29.204 30.153 34.696 35.699 36.119 36.689 36.889 35.717	-2.041 -2.918 4.397 5.625 5.892 5.834 6.859 6.845 6.312 8.224 6.093 6.337 7.800 8.253 8.459 8.532	1.00 64.65 1.00 65.94 1.00 56.58 1.00 55.58 1.00 52.46 1.00 50.69 1.00 49.69 1.00 53.46 1.00 53.94 1.00 53.94 1.00 53.46 1.00 53.76 1.00 48.07 1.00 44.87 1.00 44.81 1.00 43.13 1.00 43.13
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	544 545 546 547 549 551 552 555 555 555 555 556 556 556 556 556	CE2 CZ OH N CA C O CB CG CD1 CA C C O CB N CA C C C C C C C C C C C C C C C C C	TYR 1 TYR 1 LEU 1 LEU 1 LEU 1 LEU 1 LEU 1 LEU 1 ALA 1 ALA 1 ALA 1 ILE 1 ILE 1	8 899 8 899 8 899 8 900 8 900 8 900 8 900 8 900 8 900 8 901 8 901 8 901 8 901 8 901 8 901 8 902 8 902	19.395 20.089 17.269 17.006 18.209 19.359 15.786 16.449 15.211 17.923 18.972 18.893 17.895 18.777 19.919 20.012	29.384 28.577 31.750 32.506 33.421 30.472 29.204 30.153 34.696 35.699 36.899 36.899 36.899 35.717 35.929	-2.041 -2.918 4.397 5.625 5.892 5.834 6.859 6.845 6.312 8.224 6.093 6.337 7.800 8.253 5.429 8.532 9.979	1.00 64.65 1.00 65.94 1.00 56.58 1.00 56.58 1.00 52.46 1.00 50.69 1.00 52.94 1.00 53.02 1.00 53.02 1.00 53.76 1.00 48.07 1.00 48.07 1.00 42.43 1.00 42.43 1.00 43.13 1.00 42.59 1.00 42.59 1.00 42.59
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	544 545 546 547 548 555 555 555 555 555 556 555 5	CE2 CZ OH N CA C O CB CG CD1 CA C C O CB N CA C C C C C C C C C C C C C C C C C	TYR 1 TYR 1 LEU 1 LEU 1 LEU 1 LEU 1 LEU 1 LEU 1 ALA 1 ALA 1 ALA 1 ILE 1 ILE 1	8 8 9 9 8 8 9 9 8 8 9 9 9 0 0 8 9 0 0 0 8 9 0 0 0 8 9 0 0 0 8 9 0 0 1 8 9 0 0 1 8 9 0	19.395 20.089 17.269 17.006 18.209 19.359 16.742 15.786 16.449 15.211 17.923 18.972 18.893 17.895 18.777 19.919 20.012 20.926	29.384 28.577 31.750 32.506 33.421 33.002 31.664 30.472 29.204 30.153 34.696 35.699 36.119 36.899 35.717 35.929 37.088	-2.041 -2.918 4.397 5.625 5.892 5.834 6.859 6.845 6.312 8.224 6.093 6.337 7.800 8.253 5.429 8.532 9.979	1.00 64.65 1.00 65.94 1.00 56.58 1.00 55.58 1.00 52.46 1.00 52.94 1.00 52.94 1.00 52.94 1.00 53.05 1.00 49.63 1.00 53.76 1.00 44.87 1.00 44.87 1.00 44.87 1.00 44.87 1.00 44.83 1.00 42.43 1.00 42.59 1.00 40.02 1.00 40.02
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	544 545 546 547 549 555 555 555 555 555 555 556 560 562 563	CE2 CZ OH N CA C O CB CG CD1 CA C O CB CA C O CB CO	TYR 1 TYR 1 TYR 1 LEU 1 LEU 1 LEU 1 LEU 1 LEU 1 ALA 1 ALA 1 ALA 1 ILE 1 ILE 1 ILE 1	8 8 9 9 8 8 9 9 8 8 9 9 9 0 0 8 9 0 0 0 8 9 0 0 0 8 9 0 0 0 8 9 0 0 0 8 9 0 0 1 8 9 0	19.395 20.089 17.269 17.006 18.209 19.359 16.742 15.786 16.449 15.211 17.923 18.893 17.895 18.777 19.919 20.012 20.926 21.844	29.384 28.577 31.750 32.506 33.421 33.002 31.664 30.153 34.696 36.119 36.689 36.119 36.899 37.413	-2.041 -2.918 4.397 5.625 5.892 5.859 6.859 6.845 6.312 8.224 6.093 6.397 7.800 8.253 5.429 9.599 10.334 9.593	1.00 64.65 1.00 66.91 1.00 66.81 1.00 56.88 1.00 52.46 1.00 50.69 1.00 49.05 1.00 53.02 1.00 53.02 1.00 53.02 1.00 48.07 1.00 42.43 1.00 42.43 1.00 42.43 1.00 42.13 1.00 42.13 1.00 42.13 1.00 42.13 1.00 42.13 1.00 42.13
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	544 545 546 547 548 555 555 555 555 555 556 555 5	CE2 CZ OH N CA C O CB CG CD1 CA C C O CB N CA C C C C C C C C C C C C C C C C C	TYR 1 TYR 1 LEU 1 LEU 1 LEU 1 LEU 1 LEU 1 LEU 1 ALA 1 ALA 1 ALA 1 ILE 1 ILE 1 ILE 1 ILE 1	8 8 9 9 8 8 9 9 8 8 9 9 9 0 0 0 0 0 0 0	19.395 20.089 17.269 17.006 18.209 19.359 16.742 15.786 16.449 15.211 17.923 18.972 18.893 17.895 18.777 19.919 20.012 20.926	29.384 28.577 31.750 32.506 33.421 33.002 31.664 30.472 29.204 30.153 34.696 35.699 36.119 36.899 35.717 35.929 37.088	-2.041 -2.918 4.397 5.625 5.892 5.834 6.859 6.845 6.312 8.224 6.093 6.337 7.800 8.253 5.429 8.532 9.979	1.00 64.65 1.00 65.94 1.00 56.58 1.00 55.58 1.00 52.46 1.00 52.94 1.00 52.94 1.00 52.94 1.00 53.05 1.00 49.63 1.00 53.76 1.00 44.87 1.00 44.87 1.00 44.87 1.00 44.87 1.00 44.83 1.00 42.43 1.00 42.59 1.00 40.02 1.00 40.02

ATOM	566	CG2	ILE :	R	902	20.538	34.742	12.152	1.00 38.02
ATOM	567		ILE			18.288	33.542	10.392	1.00 44.70
ATOM	568		GLU		903	20.702	37.692	11.498	1.00 38.24
			GLU		903	21.487	38.756	12.058	1.00 36.51
MOTA	569		GLU		903	22.929	38.231	12.121	1.00 37.45
ATOM	570		GLU		903	23.188	37.096	12.569	1.00 37.05
ATOM	571					20.984	39.024	13.484	1.00 36.53
ATOM	572		GLU		903		39.865	14.343	1.00 39.44
ATOM	573		GLU		903	21.936			1.00 40.57
ATOM	574		GLU		903	21.384	40.070	15.735	1.00 40.57
ATOM	575		GLU		903	21.848	40.909	16.534	
ATOM	576		GLU		903	20.387	39.361	16.065	1.00 39.59
ATOM	577	N	TYR	В	904	23.817	39.039	11.558	1.00 36.26
ATOM	578	CA	TYR	В	904	25.236	38.729	11.507	1.00 38.11
ATOM	579	С	TYR	В	904	25.928	39.016	12.842	1.00 36.13
ATOM	580	0	TYR	В	904	25.810	40.085	13.447	1.00 36.04
ATOM	581	CB	TYR	В	904	25.870	39.456	10.293	1.00 38.03
ATOM	582	CG	TYR	В	904	27.340	39.121	10.159	1.00 39.56
ATOM	563	CD1	TYR	В	904	27.790	37.827	9.900	1.00 40.02
ATOM	584	CD2	TYR	В	904	28.296	40.122	10.364	1.00 39.80
ATOM	585		TYR	В	904	29.154	37.532	9.822	1.00 40.07
ATOM	586		TYR		904	29.641	39.846	10.258	1.00 39.30
ATOM	587	CZ	TYR		904	30.043	38.571	9.994	1.00 38.67
ATOM	588	OH	TYR		904	31.395	38.341	9.943	1.00 42.02
ATOM	589	N	ALA		905	26.565	37.994	13.427	1.00 33.70
ATOM	590	CA	ALA		905	27.351	38.148	14.629	1.00 34.04
ATOM	591	C	ALA		905	28.807	38.331	14.173	1.00 34.59
ATOM	592	ō	ALA		905	29.422	37.413	13.631	1.00 34.61
ATOM	593	CB	ALA		905	27.272	36.924	15.544	1.00 31.52
ATOM	594	N	PRO		906	29.362	39.523	14.313	1.00 37.23
ATOM	595	CA	PRO		906	30.702	39.735	13.790	1.00 36.90
ATOM	596	C	PRO		906	31.854	39.167	14.554	1.00 37.30
ATOM	597	ō	PRO		906	32.998	39.226	14.071	1.00 37.05
MOTA	598	CB	PRO		906	30.757	41.248	13.601	1.00 38.72
ATOM	599	CG		В	906	29.641	41.840	14.378	1.00 39.46
	600	CD	PRO		906	28.736	40.738	14.854	1.00 35.60
MOTA	601	N	HIS		907	31.720	38.652	15.767	1.00 35.76
MOTA		CA	HIS		907	32.810	38.072	16.515	1.00 34.45
ATOM	602	C	HIS		907	32.768	36.551	16.532	1.00 33.29
ATOM	603	0	HIS			33.420	36.044	17.429	1.00 36.68
ATOM	604	CB			907	32.793	38.614	17.971	1.00 32.90
ATOM	605	CG			907	32.706	40.082	17.966	1.00 33.20
ATOM	606					33.802	40.846	17.590	1.00 35.03
ATOM	607	ND1			907	31.727	40.985	18.200	1.00 31.98
MOTA	608	CD2	HIS		907	33.497	42.128	17.610	1.00 33.06
ATOM	609		HIS				42.128	18.017	1.00 33.02
ATOM	610		HIS			32.241	35.804	15.757	1.00 30.48
MOTA	611	N			908	32.021	34.380	15.765	1.00 32.68
ATOM	612	CA			908	32.010		16.838	1.00 31.58
ATOM	613	C	GLY			31.084	33.774		1.00 28.30
ATOM	614	0	GLY			30.218	34.407	17.431	1.00 27.49
MOTA	615	N	ASN			31.300	32.477	17.068	1.00 27.49
MOTA	616	CA	ASN			30.550	31.793	18.108	1.00 25.93
MOTA	617	C	ASN			31.321	32.036	19.407	
ATOM	618	0	ASN			32.485	32.498	19.367	1.00 28.49
ATOM	619	CB	ASN			30.241	30.343	17.894	1.00 26.09
ATOM	620	CG	ASN			31.306	29.286	17.946	
ATOM	621		ASN			31.088		17.867	1.00 30.89
ATOM	622	ND2	ASN	E	909	32.526	29.772	18.045	1.00 25.36

ATOM	523	N	LEU		910	30.721	31.746	20.545	1.00 23.98
ATOM	624	CA	LEU	В	910	31.369	32.013	21.809	1.00 24.27
ATOM	625	C	LEU	В	910	32.494	31.025	22.149	1.00 28.34
ATOM	626	0	LEU	В	910	33.475	31.482	22.740	1.00 28.22
ATOM	627	CB	LEU	В	910	30.268	31.885	22.850	1.00 22.33
ATOM	628	CG	LEU	В	910	30.701	31.957	24.327	1.00 23.69
ATOM	629	CD1	LEU	В	910	31.394	33.213	24.683	1.00 22.29
ATOM	630	CD2	LEU	В	910	29.417	31.790	25.166	1.00 21.67
ATOM	631	N	LEU	В	911	32.290	29.750	21.805	1.00 27.95
ATOM	632	CA	LEU	В	911	33.380	28.801	22.034	1.00 25.73
ATOM	633	С	LEU	В	911	34.638	29.295	21.337	1.00 27.49
ATOM	634	0	LBU		911	35.676	29.359	22.043	1.00 26.42
ATOM	635	CB	LEU	В	911	33.003	27.396	21.533	1.00 27.05
ATOM	636	CG		В	911	34.062	26.292	21.771	1.00 25.84
ATOM	637	CD1	LEU		911	34.319	26.301	23.302	1.00 20.85
ATOM	638	CD2	LEU		911	33.505	24.899	21.410	1.00 23.88
ATOM	639	N	ASP		912	34.686	29.509	20.034	1.00 27.48
ATOM	640	CA		В	912	35.832	30.077	19.341	1.00 30.26
ATOM	641	C		В	912	36.323	31.426	19.869	1.00 30.20
ATOM	642	ō		В	912	37.540	31.426	19.938	1.00 29.65
ATOM	643	CB	ASP		912	35.557	30.313		
ATOM	644	CG	ASP		912	35.339	29.102	17.848 16.995	
ATOM		OD1							1.00 34.53
	645		ASP		912	34.882	29.274	15.841	1.00 37.84
ATOM	646	OD2	ASP		912	35.663	27.975	17.416	1.00 37.21
ATOM	647	N	PHE		913	35.440	32.298	20.355	1.00 31.78
ATOM	648	CA	PHE		913	35.763	33.564	20.967	1.00 29.21
ATOM	649	C		В	913	36.507	33.319	22.291	1.00 30.28
ATOM	650	0	PHE		913	37.612	33.931	22.463	1.00 27.63
ATOM	651	CB	PHE		913	34.591	34.492	21.208	1.00 27.45
ATOM	652	CG	PHE		913	34.831	35.958	21.499	1.00 29.93
ATOM	653	CD1	PHE		913	35.060	36.840	20.461	1.00 28.75
ATOM	654	CD2	PHE		913	34.910	36.415	22.816	1.00 27.43
ATOM	655	CE1		В	913	35.313	38.202	20.715	1.00 28.06
ATOM	656	CE2		В	913	35.188	37.763	23.068	1.00 29.46
ATOM	657	CZ	PHE		913	35.379	38.643	22.029	1.00 28.47
ATOM	658	N	LEU		914	36.054	32.404	23.151	1.00 26.55
ATOM	659	CA	LEU	В	914	36.844	32.188	24.365	1.00 31.20
ATOM	660	C	LEU	В	914	38.154	31.425	24.075	1.00 30.42
ATOM	661	0	LEU	В	914	39.065	31.539	24.890	1.00 29.64
ATOM	662	CB	LEU	₿	914	36.133	31.379	25.440	1.00 32.99
ATOM	663	CG	LEU	В	914	34.718	31.897	25.858	1.00 32.39
ATOM	664	CD1	LEU	В	914	33.745	30.794	26.190	1.00 31.43
ATOM	665	CD2	LEU	В	914	34.981	32.805	27.062	1.00 27.44
ATOM	666	N	ARG	В	915	38.196	30.595	23.029	1.00 28.43
ATOM	667	CA	ARG	В	915	39.414	29.824	22.755	1.00 29.31
ATOM	668	C	ARG	В	915	40.498	30.753	22.149	1.00 32.00
ATOM	669	0	ARG		915	41.692	30.583	22.478	1.00 33.32
ATOM	670	CB	ARG		915	39.157	28.572	21.911	1.00 25.22
ATOM	671	CG	ARG		915	38.723	27.348	22.800	1.00 24.37
ATOM	672	CD	ARG		915	38.161	26.209	21.957	1.00 24.37
ATOM	673	NE	ARG		915	37.642	25.132	22.889	1.00 26.89
ATOM	674	CZ	ARG		915	37.100	24.031	22.346	1.00 25.09
ATOM	675	NH1	ARG		915	37.100	23.901	21.016	1.00 25.09
ATOM	676	NH2	ARG		915	36.588	23.301	23.194	1.00 24.19
ATOM	677	Nnz		В	916	40.164	31.751	23.194	1.00 23.94
ATOM	678	CA	LYS		916	40.164	32.736	20.705	1.00 34.12
ATOM	679	C	LYS		916				
ATOM	0/2	_	nis	Ð	210	41.664	33.693	21.683	1.00 36.01

ATOM	680	٥	LYS	B	916	42.762	34.252	21.536	1 00	36.61
ATOM	681	CB	LYS			40.287	33.552	19.615		34.37
ATOM	682	CG	LYS		916	40.129	32.825	18.298		42.16
	683	CD	LYS			39.443	33.575	17.172		44.43
ATOM		CE	LYS		916	38.756	32.732	16.114		47.47
ATOM	684	NZ	LYS			37.371	33.261	15.814		51.77
ATOM	685							22.786		33.46
MOTA	686	N	SER			40.991	33.857			
ATOM	687	CA	SER		917	41.419	34.647	23.937		32.01
ATOM	688	C	SER		917	42.545	34.012	24.721		32.62
ATOM	689	0	SER		917	43.188	34.725	25.520		27.96
ATOM	690	CB	SER		917	40.117	34.800	24.689		31.09
ATOM	691	OG	SER		917	40.057	34.497	26.054		33.24
MOTA	692	N	ARG		918	42.926	32.735	24.574		33.26
ATOM	693	CA	ARG			43.911	32.087	25.401		29.88
ATOM	694	C	ARG		918	45.341	32.471	24.927		33.33
MCTA	695	0	ARG		918	46.072	31.782	24.226		34.36
MOTA	696	CB	ARG	В	918	43.750	30.570	25.487	1.00	30.84
ATOM	697	CG	ARG	В	918	42.350	30.118	25.969	1.00	31.53
ATOM	698	CD	ARG	В	918	42.301	28.655	26.234	1.00	31.59
ATOM	699	NE	ARG	В	918	41.373	27.771	26.776	1.00	30.40
ATOM	700	CZ	ARG	В	918	41.314	26.510	27.146	1.00	27.78
ATOM	701	NH1	ARG	В	918	42.579	25.901	27.032	1.00	24.30
ATOM	702	NH2	ARG	В	918	40.359	25.804	27.635	1.00	24.57
ATOM	703	N	VAL	В	919	45.792	33.639	25.388	1.00	29.19
ATOM	704	CA	VAL	в	919	46.914	34.362	24.991	1.00	31.89
ATOM	705	С	VAL			48.324	33.779	25.390	1.00	33.48
ATOM	706	o	VAL			49.318	34.428	25.239		42.15
ATOM	707	CB	VAL			47.064	35.854	25.366	1.00	30.88
ATOM	708		VAL			46.027	36.669	24.602		34.82
MOTA	709	CG2				46.881	36.061	26.852	1.00	31.88
ATOM	710	N	LEU			48.272	32.609	25.986		31.42
MOTA	711	CA	LEU			49.386	31.803	26.310		32.43
MOTA	712	C	LEU			49.646	30.949	25.049		33.59
ATOM	713	ō	LEU			50.874	30.754	24.757		34.43
ATOM	714	CB	LEU			49.363	30.892	27.516		26.98
MOTA	715	CG	LEU			49.473	31.646	28.827		28.45
ATOM	716		LEU			49.060	30.712	29.911		24.11
MOTA	717	CD2	LEU			50.899	32.259	29.084		24.38
ATOM	718	N	GLU			48.560	30.587	24.414		33.03
ATOM	719	CA	GLU			48.691	29.839	23.163		34.88
ATOM	720	C	GLU			48.686	30.741	21.960		36.44
ATOM	721	ō	GLU			49.468	30.532	21.028		37.60
ATOM	722	CB	GLU			47.526	28.797	23.034		36.48
ATOM	723	ĊG	GLU			47.367	28.228	21.636		39.16
ATOM	724	CD	GLU			46.213	27.255	21.414		43.37
ATOM	725	OE1	GLU			45.489	26.854	22.357		41.90
							26.848			42.19
ATOM	726	OE2	GLU			46.044		20.222		
ATOM	727	N	THR			47.772	31.738	21.886		33.22
ATOM	728	CA	THR			47.684	32.482	20.652		33.16
MOTA	729	C	THR			48.566	33.711	20.605		33.32
MOTA	730	0	THR			48.787	34.124	19.452		33.82
ATOM	731	CB	THR			46.212	32.897	20.346		33.96
ATOM	732	OG1	THR			45.814	33.744	21.415		33.38
MOTA	733	CG2	THR			45.288	31.667	20.363		35.79
ATOM	734	N	ASP	В		49.134	34.252	21.645		34.17
ATOM	735	CA	ASP			50.099	35.410	21.445		33.90
ATOM	736	C	ASP	В	923	50.855	35.464	22.736	1.00	31.06

Nancy J. Bump et al.

50.593 36.342 23.567 1.00 27.46

49.307 36.710 21.268 1.00 37.04

20.960 1.00 41.38

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ATOM

ATOM

ATOM

792 CA SER B 931

SER B 931

793 C

ATOM

ATOM

737 C

738 CB

ASP B 923

ASP B 923

51.064 39.195 32.863 1.00 34.73

49.616 38.647 32.909 1.00 31.81

ATOM	794	0	SER	В	931	48.946	38.522	33.960	1.00	28.51
ATOM	795	CB	SER		931	51.539	39.966	34.083		36.38
ATOM	796	OG	SER	В	931	51.372	39.137	35.239	1.00	44.81
ATOM	797	N	THR	В	932	49.066	38.367	31.708	1.00	31.32
MOTA	798	CA	THR		932	47.681	37.822	31.741		33.33
ATOM	799	C			932	47.532	36.490	31.036		31.10
ATOM	800	0	THR		932	48.276	36.141	30.127		30.68
ATOM	801	CB	THR		932	46.678	38.870	31.263		33.87
ATOM	802	OG1	THR	В	932	45.316	38.426	31.576		33.49
ATOM	803	CG2	THR		932	46.692	39.109	29.757		33.71
ATOM	804	N	ALA		933	46.529	35.668	31.389		31.61
ATOM	805	CA	ALA		933	46.226	34.431	30.705		29.07
ATOM	806	C	ALA		933	45.091	34.589	29.655		30.40
ATOM	807	0	ALA		933	44.908	33.676	28.853		28.66
ATOM	808	CB	ALA		933	45.737	33.378	31.703		27.24
ATOM	809	N	SER		934	44.450	35.779	29.587		26.77
ATOM	810	CA	SER		934	43.413	36.013	28.587		28.62
ATOM	811	C	SER		934	43.413	37.464	28.195		27.31
ATOM	812	0	SER		934	43.323	38.417	28.980		27.55
ATOM	813	CB	SER		934	42.064	35.455	29.162		26.81
	814	OG	SER		934	42.084	35.744	28.323		27.56
ATOM					934	42.820	37.745	26.944		27.99
ATOM	815	N	THR					26.578		29.68
MOTA	816	CA		В	935	42.439	39.110	27.282		31.68
ATOM	817	C	THR		935	41.160	39.524			
MOTA	818	0	THR		935	40.842	40.718	27.320		33.62
MOTA	819	CB	THR		935	42.242	39.350	25.075		
ATOM	820	OG1	THR		935	41.506	38.262	24.505		29.66
ATOM	821	CG2	THR		935	43.525	39 478	24.287		30.00
ATOM	822	N	LEU	В	936	40.343	38.579	27.771		31.45
MOTA	823	CA	LEU		936	39.018	38.902			29.86
MOTA	824	C	LEU		936	39.137	39.093	29.820		28.85
ATOM	825	0	LEU		936	39.947	38.339			35.21
ATOM	826	CB	LEU	В	936	38.171	37.634	28.127		38.52
ATOM	827	CG	LEU		936	37.312	37.342	26.944		
ATOM	828	CD1	LEU		936	37.602	38.053	25.641		42.04
ATOM	829	CD2	LEU		936	37.181	35.833	26.689		40.21
MOTA	830	N	SER		937	38.381	39.888	30.508	1.00	
ATOM	831	CA	SER		937	38.427	39.976	31.975		27.30
ATOM	832	C		В	937	37.373	39.107	32.612	1.00	25.12
ATOM	833	0	SER		937	36.444	38.641			28.29
ATOM	834	CB	SER		937	38.164	41.408	32.478		
ATOM	835	OG	SER		937	36.753	41.746	32.275		26.99
MOTA	836	N		В	938	37.382	38.946	33.936	1.00	
ATOM	837	CA	SER		938	36.444	38.301	34.738	1.00	25.14
ATOM	838	C	SER		938	34.982	38.781	34.508		29.67
ATOM	839	0	SER		938	33.973	38.052	34.324		28.12
ATOM	840	CB	SER		938	36.842	38.693	36.180		25.42
ATOM	841	OG	SER		938	35.935	37.879	36.971	1.00	
ATOM	842	N	GLN		939	34.834	40.109	34.487		27.93
ATOM	843	CA	GLN		939	33.576	40.797	34.290	1.00	
ATOM	844	C	GLN		939	33.036	40.463	32.911		26.11
ATOM	845	0	GLN	В	939	31.840	40.271	32.714		28.65
ATOM	846	CB	GLN	В	939	33.784	42.330	34.312	1.00	
ATOM	847	CG	GLN		939	33.442	43.229	35.457		40.59
ATOM	848	CD	GLN		939	32.130	43.133	36.180		39.70
ATOM	849	OE1	GLN	В	939	31.005	43.468	35.831	1.00	47.06

TO CHILDREN COLUMN

32.185 42.646 37.424 1.00 42.39

850 NE2 GLN B 939

ATOM

ATOM	851	N	GLN B	940	33.893	40.437	31.879	1.00 28.10
ATOM	852	CA.	GLN B	940	33.294	39.992	30.590	1.00 26.42
ATOM	853	C	GLN B	940	32.792	38.510	30.608	1.00 27.93
ATOM	954	0	GLN B	940	31.699	38.213	30.003	1.00 24.42
MOTA	855	CB	GLN B	940	34.237	40.315	29.474	1.00 28.32
ATOM	856	CG	GLN B	940	33.821	39.728	28.138	1.00 30.12
MCTA	857	CD	GLN B	940	32.714	40.351	27.341	1.00 32.84
ATOM	858	OE1	GLN B	940	32.980	40.952	26.293	1.00 32.97
ATOM	859	NE2	GLN B	940	31.444	40.215	27.742	1.00 32.92
ATOM	860	N	LEU B	941	33.469	37.651	31.370	1.00 26.91
MOTA	861	CA	LEU B	941	32.909	36.258	31.443	1.00 28.19
MOTA	862	C	LEU B	941	31.589	36.301	32.198	1.00 29.57
ATOM	863	С	LEU B	941	30.678	35.590	31.730	1.00 30.43
ATOM	864	CB	LEU B	941	33.906	35.296	32.049	1.00 25.27
ATOM	865	CG	LEU B	941	35.315	35.323	31.415	1.00 32.42
ATOM	866	CD1	LEU B	941	36.323	34.485	32.227	1.00 31.29
ATOM	867	CD2	LEU B	941	35.341	34.767	30.010	1.00 31.88
ATOM	868	74	LEU B	942	31.450	37.064	33.293	1.00 30.31
ATOM	869	CA	LEU B	942	30.167	37.145	33.968	1.00 32.16
ATOM	870	C	LEU B	942	29.036	37.749	33.115	1.00 31.83
ATOM	871	0	LEU B	942	27.922	37.185	33.174	1.00 33.88
ATOM	872	CB	LEU B	942	30.243	37.957	35.236	1.00 31.72
ATOM	873	CG	LEU B	942	31.083	37.434	36.382	1.00 33.04
MOTA	874	CD1	LEU B	942	31.284	38.550	37.417	1.00 33.30
ATOM	875	CD2	LEU B	942	30.573	36.187	36.999	1.00 35.60
ATOM	876	N	HIS B	943	29.333	38.722	32.292	1.00 30.14
ATOM	877	CA	HIS B	943	28.489	39.305	31.307	1.00 32.55
ATOM	878	C	HIS B	943	27.988	38.261	30.293	1.00 33.04
MOTA	879	0	HIS B	943	26.773	38.281	29.997	1.00 29.13
ATOM	880	CB	HIS B	943	29.051	40.525	30.513	1.00 31.92
ATOM	881	CG	HIS B	943	28.919	41.826	31.219	1.00 34.62
ATOM	882		HIS B	943	29.954	42.688	31.481	1.00 36.03
ATOM	883	CD2	HIS B	943	27.832	42.442	31.778	1.00 38.05
ATOM	884	CE1	HIS B		29.547	43.737	32.168	1.00 35.60
ATOM	885	NE2	HIS B	943	28.245	43.626	32.354	1.00 37.32
ATOM	886	N	PHE B	944	28.860	37.419	29.710	1.00 30.43
ATOM	887	CA	PHE B	944	28.322	36.430	28.793	1.00 30.42
ATOM	888	C	PHE B	944	27.361	35.447	29.480	1.00 28.35
ATOM	889	0	PHE B	944	26.297	35.095	28.948	1.00 27.55
ATOM	890	CB	PHE B	944	29.414	35.601	28.129	1.00 29.40
ATOM	891	CG	PHE B	944	30.259	36.326	27.143	1.00 28.28
ATOM	892	CD1	PHE B	944	31.639	36.118	27.152	1.00 28.85
ATOM	893	CD2	PHE B	944	29.764	37.193	26.200	1.00 27.36
ATOM	894	CE1	PHE B	944	32.429	36.783	26.230	1.00 31.22
ATOM	895	CE2	PHE B	944	30.528	37.861	25.279	1.00 30.76
ATOM	896	CZ	PHE B	944	31.863	37.640	25.305	1.00 29.54
ATOM	897	N	ALA B	945	27.661	35.064	30.707	1.00 28.20
ATOM	898	CA	ALA B	945	26.737	34.232	31.526	1.00 27.06
ATOM	899	C	ALA B	945	25.389	34.896	31.781	1.00 28.16
ATOM	900	0	ALA B	945	24.305	34.272	31.603	1.00 29.72
ATOM	901	CB	ALA B	945	27.424	33.982	32.882	1.00 22.24
ATOM	902	N	ALA B	946	25.348	36.185	32.154	1.00 28.40
ATOM	903	CA	ALA B	946	24.058	36.906	32.424	1.00 26.80
ATOM	904	C	ALA B	946	23.326	37.071	31.128	1.00 26.73
ATOM ATOM	905 906	O CB	ALA B	946 946	22.095	36.826	30.960	1.00 33.16
ATOM	908	N	ASP B		24.422	38.268		
ATOM	90/	TA.	ADF B	94/	24.021	37.501	30.077	1.00 25.12

CONTROL COUNTY

Docket/App No.: 2079.1037-001

Title: Method of Identifying Inhibitors of TIE-2 Inventors: Nancy J. Bump et al.

ATOM	908	CA	ASP B	947	23.361	37.562	28.793	1.00 27.64
ATOM	909	C	ASP B	947	22.653	36.217	28.522	1.00 30.15
ATOM	910	0	ASP B	947	21.423	36.331	28.285	1.00 32.77
ATOM	911	CB	ASP B	947	24.158	37.947	27.594	1.00 32.32
ATOM	912	CG	ASP B	947	24.798	39.318	27.538	1.00 37.39
	913		ASP B	947	24.327	40.283	28.209	1.00 38 95
ATOM	914	OD2	ASP B	947	25.817	39.462	26.816	1.00 38.99
ATOM	915	N	VAL B	948	23.225	35.043	28.511	1.00 24.93
ATOM ATOM	916	CA	VAL B	948	22.519	33.824	28.235	1.00 26.37
		CA	VAL B	948	21.319	33.657	29.150	1.00 26.38
ATOM ATOM	917 918	0	VAL B	948	20.273	33.241	28.688	1.00 28.00
		CB	VAL B	948	23.423	32.575	28.375	1.00 23.63
ATOM ATOM	919 920	CGl	VAL B	948	22.711	31.247	28.218	1.00 28.41
ATOM	921	CG2	VAL B	948	24.500	32.621	27.306	1.00 24.29
ATOM	921	N N	ALA B	949	21.496	33.853	30.472	1.00 25.90
	923	CA	ALA B	949	20.489	33.633	31.449	1.00 24.76
ATOM	924	C	ALA B	949	19.254	34.514	31.245	1.00 29.82
ATOM		0	ALA B	949	18.125	33.995	31.478	1.00 29.12
ATOM	925	CB	ALA B	949	21.105	33.945	32.833	1.00 23.12
MOTA	926		ARG B	950	19.483	35.753	30.814	1.00 29.05
ATOM	927	N CA	ARG B	950	19.463	36.711	30.514	1.00 29.74
ATOM	928	CA	ARG B	950	17.681	36.245	29.315	1.00 30.35
ATOM	929		ARG B	950	16.454	36.156	29.291	1.00 32.30
MOTA	930	0	ARG B	950	18.943	38.135	30.331	1.00 29.04
MOTA	931	CB	ARG B	950	17.857	39.209	30.253	1.00 29.74
ATOM	932	CD	ARG B	950	18.484	40.540	29.840	1.00 33.11
ATOM	933 934	NE	ARG B	950	19.702	40.789	30.623	1.00 36.26
ATOM	935	CZ	ARG B	950	20.973	41.064	30.349	1.00 36.47
ATOM ATOM	936		ARG B	950	21.905	41.281	31.276	1.00 34.51
	935		ARG B	950	21.303	41.281	29.088	1.00 37.31
ATOM ATOM	937	NH2 N	GLY B		18.419	35.817	28.306	1.00 29.52
ATOM	939	CA	GLY B		17.811	35.222	27.135	1.00 30.22
ATOM	940	C	GLY B		16.981	34.005	27.518	1.00 31.96
ATOM	941	0	GLY B		15.802	33.895	27.083	1.00 30.42
ATOM	942	N	MET B		17.505	33.082	28.335	1.00 31.58
ATOM	943	CA	MET B		16.833	31.858	28.668	1.00 31.52
ATOM	944	C	MET B		15.593	32.060	29.545	1.00 31.14
ATOM	945	Ö	MET B		14.692	31.277	29.453	1.00 32.05
ATOM	946	CB	MET B		17.728	30.817	29.348	1.00 32.91
ATOM	947	CG	MET B		18.601	29.963	28.470	1.00 28.12
ATOM	948	SD	MET E		17.803	29.220	27.056	1.00 28.47
ATOM	949	CE	MET E		16.601	28.118	27.850	1.00 24.09
ATOM	950	N	ASP E		15.540	32.991	30.425	1.00 33.12
ATOM	951	CA	ASP E		14.479	33.295	31.364	1.00 35.52
ATOM	952	C	ASP E		13.331	33.873	30.536	1.00 34.51
ATOM	953	0	ASP E		12.167	33.463	30.579	1.00 34.88
ATOM	954	CB	ASP E		14.959	34.196	32.470	1.00 37.38
ATOM	955	CG	ASP E		13.886	35.033	33.182	1.00 38.60
ATOM	956	OD1			13.235	34.579	34.136	1.00 38.16
ATOM	957	OD2			13.774	36.209	32.830	1.00 39.51
ATOM	958	N		954	13.741	34.680	29.561	1.00 34.22
ATOM	959	CA	TYR E		12.764	35.208	28.602	1.00 33.92
ATOM	960	C	TYR E		12.083	34.027	27.920	1.00 35.03
ATOM	961	0	TYR I		10.854	33.911	27.879	1.00 33.83
ATOM	962	CB	TYR I		13.457	36.158	27.672	1.00 36.04
MOTA	963	CG	TYR I	954	12.621	36.621	26.523	1.00 40.14
ATOM	964	CD3			11.489	37.372	26.834	1.00 42.51

ATOM	965	CD2	TYR	В	954	12.873	36.322	25.202	1.00	40.08
ATOM	966		TYR		954	10.587	37.819	25.869	1.00	45.17
ATOM	967	CE2	TYR		954	12.012	36.762	24.225	1.00	44.28
MOTA	968	CZ	TYR	В	954	10.893	37.541	24.548	1.00	45.99
ATOM	969	OH	TYR	В	954	10.043	37.968	23.564		46.72
ATOM	970	N	LEU	В	955	12.809	33.080	27.399		34.55
ATOM	971	CA	LEU		955	12.388	31.912	26.704		34.31
MOTA	972	C	LEU		955	11.690	30.956	27.654		32.95
MOTA	973	0	LEU		955	10.537	30.633	27.336		36.79
MOTA	974	CB	LEU		955	13.431	31.053	26.006		34.82
MOTA	975	CG	LEU		955	14.032	31.673	24.757		30.87
MOTA	976		LEU		955	15.304	30.976	24.341		32.89
ATOM	977	CD2	LEU		955	13.075	31.726 30.620	28.798		33.38
ATOM	978	N	SER		956 956	12.231 11.489	29.672	29.609		34.02
ATOM	979 980	CA C	SER		956	10.214	30.243	30.247		34.18
ATOM ATOM	981	0	SER		956	9.393	29.419	30.652		30.24
ATOM	982	CB	SER			12.469	29.126	30.630		33.64
MOTA	983	OG	SER		956	12.613	30.134	31.586		37.17
ATOM	984	N	GLN			10.032	31.530	30.438		32.94
ATOM	985	CA	GLN		957	8.852	32.137	31.059	1.00	37.57
ATOM	986	C	GLN		957	7.675	32.048	30.084	1.00	36.65
MOTA	987	0	GLN	В	957	6.518	31.962	30.443	1.00	36.69
ATOM	988	CB	GLN		957	9.101	33.516	31.671	1.00	39.36
ATOM	989	CG	GLN	В	957	9.819	33.491	33.028	1.00	43.44
ATOM	990	CD	GLN	В	957	10.305	34.801	33.581	1.00	47.63
ATOM	991	OE1	GLN	В	957	10.420	35.138	34.789	1.00	48.94
ATOM	992	NE2	GLN	В	957	10.736	35.802	32.807		50.75
ATOM	993	N	LYS	В	958	7.937	31.933	28.792		37.29
ATOM	994	CA	LYS		958	7.068	31.649	27.696		36.90
ATOM	995	С	LYS		958	6.830	30.166	27.402		39.87
ATOM	996	0	LYS			6.248	29.735	26.407		41.16
ATOM	997	CB	LYS		958	7.554	32.393	26.439		40.75
ATOM	998	CG	LYS		958	7.237	33.862	26.545		42.57
ATOM	999	CD	LYS	В	958	7.853	34.666 35.852	25.399 25.045		49.59
ATOM	1000	CE	LYS		958	6.950 7.755	36.850	24.277		50.56
ATOM ATOM	1001	NZ N	LYS		958 959	7.733	29.272	28.275		38.89
ATOM	1002	CA	GLN		959	7.191	27.826	28.340		39.77
ATOM	1003	C	GLN		959	7.985	27.154	27.246		36.45
ATOM	1005	0	GLN		959	7.889	25.977	26.904		34.64
ATOM	1006	CB	GLN		959	5.729	27.298	28.353	1.00	42.27
ATOM	1007	CG	GLN		959	5.062	27.411	29.706	1.00	47.02
ATOM	1008	CD			959	3.550	27.270	29.700	1.00	52.44
ATOM	1009	OE1	GLN	В	959	2.905	27.301	30.787	1.00	54.64
ATOM	1010	NE2	GLN	В	959	2.888	27.133	28.539	1.00	51.33
MOTA	1011	N	PHE	В	960	8.932	27.911	26.701		35.89
ATOM	1012	CA	PHE	В	960	9.764	27.490	25.601		34.12
ATOM	1013	C			960	11.017	26.758	26.168		34.10
ATOM	1014	0			960	11.310	27.045	27.320		36.77
MOTA	1015	CB			960	10.127	28.752	24.850		38.30
ATOM	1016	CG			960	9.381	29.131	23.626		37.64
MOTA	1017		PHE		960	8.691	30.350	23.577		39.17
MOTA	1018	CD2			960	9.322	28.313	22.534		37.83
MOTA	1019	CE1			960	7.970	30.753	22.460		38.89
ATOM	1020	CE2			960	8.612 7.938	28.711	21.415		38.28
MOTA	1021	CZ	PHE	. ¤	960	7.938	25.930	21.3/2	4.00	20.20

ATOM	1022	N	ILE B	961	11.301	25.645	25.515	1.00	32.04
ATOM	1023	CA	ILE B		12.386	24.751	25.913	1.00	35.73
ATOM	1024	C	ILE B		13.444	24.628	24.816	1.00	35.82
ATOM	1025	0	ILE B		13.170	24.025	23.764	1.00	36.60
ATOM	1026	CB	ILE B		11.866	23.322	26.185		37.85
ATOM	1020	CG1	ILE B		10.658	23.219	27.079		39.27
ATOM	1027	CG2	ILE B		12.985	22.443	26.741		41.20
ATOM	1029	CD1	ILE E		10.666	23.505	28.545		39.36
	1029	N	HIS E		14.751	24.959	25.030		33.60
ATOM	1030	CA		962	15.736	24.996	23.975		31.29
ATOM	1031	C		962	16.435	23.705	23.604		30.82
ATOM		0	HIS E		16.658	23.371	22.425		29.73
ATOM	1033				16.674	26.099	24.539		31.33
ATOM	1.034	CB	HIS E		17.589	26.596	23.457		33.97
ATOM	1035	CG			17.135	26.808	22.169		33.33
ATOM	1036		HIS E			26.881	23.499		33.27
MOTA	1037		HIS E		18.913	27.242	21.492		35.73
ATOM	1038	CEl	HIS E		18.200	27.242	22.251		29.66
ATOM	1039		HIS E		19.289		24.598		30.47
ATOM	1040	N	ARG E		16.968	23.006	24.471		33.00
MOTA	1041	CA	ARG E		17.746		23.997		36.77
ATOM	1042	С	ARG E		19.194	21.923			39.62
ATOM	1043	0	ARG E		19.889	20.887	24.004		32.77
ATOM	1044	CB	ARG E		17.204	20.679	23.551		31.62
ATOM	1045	CG	ARG I		15.815	20.172	23.935		31.53
MOTA	1046	CD	ARG I		15.128	19.404	22.847		
ATOM	1047	NE	ARG I		15.025	19.871	21.521		33.88
ATOM	1048	CZ	ARG I		15.726	19.662	20.419		37.97
ATOM	1049		ARG I		16.808	18.841	20.421		37.50
ATOM	1050	NH2	ARG E		15.341	20.285	19.289		37.35
ATOM	1051	N	ASN I		19.655	23.009	23.398		36.17
ATOM	1052	CA	ASN I		20.974	23.021	22.816		38.69
MOTA	1053	C	ASN I		21.926	24.070	23.372		36.17
ATOM	1054	0	ASN I		22.772	24.513	22.610		37.84
ATOM	1055	CB	ASN I		20.798	23.344	21.298		41.85
ATOM	1056	CG	ASN I		20.079	22.173	20.634	1.00	
ATOM	1057	OD1		964	20.319	21.037	21.043		49.94
ATOM	1058	ND2	ASN I		19.184	22.496	19.688		48.13
ATOM	1059	N		B 965	21.795	24.534	24.570		32.14
ATOM	1060	CA		B 965	22.546	25.569	25.189		33.80
ATOM	1061	C	LEU :		23.994	25.064	25.398		36.44
ATOM	1062	0	LEU :		24.144	24.390	26.421		40.41
ATOM	1063	CB		B 965	22.086	25.960	26.578		31.51
ATOM	1064	CG	LEU :		20.940	26.943	26.863		30.06
ATOM	1065	CD1	LEU :		20.731	26.975	28.363	1.00	
ATOM	1066	CD2	LEU	B 965	21.491	28.298	26.403		29.20
ATOM	1067	N	ALA		24.919	25.275	24.490		31.71
ATOM	1068	CA	ALA	B 966	26.340	24.956	24.701		29.62
ATOM	1069	C	ALA	B 966	27.144	26.139	24.175		27.97
ATOM	1070	0	ALA	B 966	26.676	26.823	23.232	1.00	
ATOM	1071	CB	ALA	B 966	26.737	23.681	23.960	1.00	
ATOM	1072	N	ALA	B 967	28.451	26.232	24.492	1.00	
ATOM	1073	CA	ALA	B 967	29.236	27.348	23.991	1.00	
ATOM	1074	C	ALA	B 967	29.357	27.432	22.481	1.00	
MOTA	1075	0	ALA	B 967	29.291	28.561	21.897	1.00	
ATOM	1076	CB	ALA	B 967	30.515	27.596	24.725	1.00	
MOTA	1077	N	ARG	B 968	29.406	26.364	21.727	1.00	30.03

COCKETAL CITED

1078 CA ARG B 968

ATOM

Docket/App No.: 2079.1037-001

Title: Method of Identifying Inhibitors of TIE-2 Inventors: Nancy J. Bump *et al.*

ATOM	1079	С	ARG	В	968	28.100	27.003	19.677	1.00	30.62
ATOM	1080	0		В	968	28.131	27.362	18.476		31.68
ATOM	1081	CB	ARG		968	29.753	25.111	19.610		29.15
ATOM	1082	CG	ARG		968	28.695	24.044	19.886		31.62
ATOM	1083	CD	ARG		968	28.941	22.658	19.226		35.47
ATOM	1084	NE		В	968	27.817	21.807	19.703		38.33
ATOM	1085	CZ	ARG		968	27.827	21.154	20.851		40.05
ATOM	1086	NH1	ARG		968	28.897	21.164	21.633		42.72
ATOM	1087	NH2		В	968	26.834	20.421	21.322		43.32
ATOM	1088	N		В	969	26.979	27.025	20.436		28.92
ATOM	1089	CA		В	969	25.710	27.429	19.810		29.20
ATOM	1090	C	ASN		969	25.291	28.803	20.297		30.35
ATOM	1091	ō			969	24.086	29.145	20.204		30.32
ATOM	1092	CB	ASN		969	24.598	26.375	20.098		25.04
ATOM	1093	CG		В	969	24.914	25.020	19.495		30.26
ATOM	1094	OD1			969	25.378	24.869	18.361		32.57
ATOM	1095	ND2	ASN		969	24.648	23.886	20.172		28.51
ATOM	1096	N	ILE		970	26.257	29.496	20.910		27.55
ATOM	1097	CA		3	970	26.015	30.841	21.418		28.82
ATOM	1098	C		В	970	26.802	31.795	20.505		29.55
ATOM	1099	0	ILE		970	27.963	31.487	20.196		27.59
ATOM	1100	СЗ	ILE		970	26.412	31.038	22.895		26.22
ATOM	1101	CG1			970	25.618	30.198	23.893		25.70
ATOM	1102	CG2	ILE		970	26.312	32.536	23.261		21.48
ATOM	1103	CD1	ILE		970	24.088	30.263	23.734		23.69
ATOM	1104	N	LEU		971	26.208	32.904	20.028		29.96
ATOM	1105	CA		В	971	26.961	33.826	19.172		30.19
ATOM	1106	C	LEU		971	27.438	35.090	19.845		31.70
ATOM	1107	ō	LEU		971	26.784	35.584	20.761		33.46
ATOM	1108	CB	LEU		971	26.085	34.128	17.930		30.67
ATOM	1109	CG			971	25.855	32.975	16.964		34.15
ATOM	1110	CD1	LEU		971	24.695	33.281	15.982		33.06
ATOM	1111	CD2	LEU		971	27.122	32.553	16.185		30.70
ATOM	1112	N	VAL		972	28.541	35.731	19.447		30.83
ATOM	1113	CA	VAL		972	29.044	36.982	20.037		32.48
ATOM	1114	C	VAL		972	28.758	38.104	19.005		30.36
ATOM	1115	ō	VAL		972	29.405	38.186	17.951		31.08
ATOM	1116	CB		В	972	30.521	36.984	20.420		32.58
ATOM	1117	CG1	VAL	В	972	30.930	38.281	21.136	1.00	34.22
ATOM	1118	CG2	VAL	В	972	30.871	35.785	21.333	1.00	31.21
ATOM	1119	N	GLY	В	973	27.711	38.847	19.310	1.00	30.33
ATOM	1120	CA	GLY	В	973	27.207	39.802	18.315	1.00	29.88
ATOM	1121	C	GLY	В	973	27.727	41.204	18.479	1.00	32.70
ATOM	1122	0	GLY	В	973	28.585	41.451	19.329	1.00	31.01
MOTA	1123	N	GLU	В	974	27.145	42.135	17.747	1.00	34.65
ATOM	1124	CA	GLU	В	974	27.522	43.527	17.855	1.00	33.72
MOTA	1125	C	GLU	В	974	27.649	43.930	19.302	1.00	33.97
ATOM	1126	0	GLU	В	974	26.870	43.530	20.180	1.00	30.31
ATOM	1127	CB	GLU	В	974	26.420	44.367	17.187	1.00	40.43
ATOM	1128	CG	GLU	В	974	26.557	44.283	15.649	1.00	48.26
ATOM	1129	CD	GLU	В	974	26.317	45.679	15.071	1.00	54.12
ATOM	1130	OEl	GLU	В	974	25.119	46.052	15.074	1.00	56.77
ATOM	1131	OE2	GLU	В	974	27.258	46.414	14.674	1.00	56.47
ATOM	1132	N	ASN	В	975	28.679	44.730	19.612	1.00	32.99
ATOM	1133	CA	ASN	В	975	28.909	45.235	20.945	1.00	32.09
ATOM	1134	C	ASN	В	975	29.202	44.081	21.877	1.00	32.69
MOTA	1135	0	ASN	В	975	29.082	44.240	23.098	1.00	33.59

ATOM	1136	CB	ASN	В	975	27.642	46.019	21.385	1.00	36.61
ATOM	1137	CG	ASN	В	975	27.446	47.285	20.540	1.00	37.11
ATOM	1138	OD3	ASN	В	975	26.276	47.739	20.363	1.00	39.26
MOTA	1139	ND2	ASN	В	975	28.530	47.826	20.042	1.00	29.86
ATOM	1140	N	TYR	В	976	29.715	42.945	21.379	1.00	32.96
ATOM	1141	CA	TYR	В	976	29.974	41.815	22.291	1.00	33.87
ATOM	1142	C	TYR	В	976	28.745	41.291	22.977	1.00	33.96
ATOM	1143	0	TYR	В	976	28.952	40.845	24.142	1.00	38.50
ATOM	1144	CB	TYR	В	976	31.090	42.145	23.319	1.00	32.57
ATOM	1145	CG	TYR	В	976	32.316	42.635	22.562	1.00	34.93
ATOM	1146	CD1	TYR	В	976	32.643	43.977	22.488	1.00	34.96
MOTA	1147	CD2	TYR	В	976	33.064	41.750	21.796	1.00	36.25
ATOM	1148	CE1	TYR	В	976	33.734	44.404	21.765	1.00	36.57
ATOM	1149	CE2	TYR	В	976	34.151	42.185	21.066	1.00	37.74
ATOM	1150	CZ	TYR	В	976	34.469	43.524	21.027	1.00	38.58
ATOM	1151	OH	TYR	В	976	35.544	43.988	20.318	1.00	41.08
ATOM	1152	N	VAL	В	977	27.498	41.318	22.583	1.00	33.38
ATOM	1153	CA	VAL	В	977	26.363	40.804	23.354	1.00	30.29
ATOM	1154	C	VAL	В	977	26.160	39.324	23.034	1.00	28.06
ATOM	1155	0	VAL	В	977	26.157	38.975	21.853	1.00	30.23
ATOM	1156	CB	VAL	В	977	25.135	41.674	23.014	1.00	29.39
ATOM	1157	CG1	VAL	В	977	23.846	41.027	23.499	1.00	28.20
ATOM	1158	CG2	VAL	В	977	25.284	43.038	23.718	1.00	31.72
ATOM	1159	N	ALA	В	978	26.159	38.459	24.028	1.00	27.76
ATOM	1160	CA	ALA	В	978	25.975	37.006	23.681	1.00	28.79
ATOM	1161	C	ALA	В	978	24.563	36.847	23.132	1.00	31.90
ATOM	1162	0	ALA	В	978	23.647	37.514	23.577	1.00	30.56
ATOM	1163	CB	ALA	В	978	26.186	36.192	24.917	1.00	25.90
ATOM	1164	N	LYS	В	979	24.330	36.043	22.103	1.00	33.62
ATOM	1165	CA	LYS	В	979	23.070	35.784	21.463	1.00	31.66
ATOM	1166	C	LYS	В	979	22.780	34.287	21.336	1.00	31.79
ATOM	1167	0	LYS	В	979	23.561	33.490	20.808	1.00	29.59
ATOM	1168	CB	LYS	В	979	23.102	36.390	20.030	1.00	34.05
ATOM	1169	CG	LYS	В	979	22.883	37.917	20.237	1.00	38.30
ATOM	1170	CD	LYS	В	979	23.149	38.766	19.049	1.00	36.22
ATOM	1171	CE	LYS	В	979	23.157	40.252	19.366	1.00	39.70
ATOM	1172	NZ	LYS	В	979	21.788	40.833	19.313	1.00	39.24
ATOM	1173	N	ILE	В	980	21.643	33.866	21.839	1.00	29.92
ATOM	1174	CA	ILE	В	980	21.279	32.444	21.718	1.00	29.31
A'TOM	1175	C	ILE	В	980	20.877	32.083	20.290	1.00	32.94
ATOM	1176	0	ILE	В	980	20.093	32.771	19.620	1.00	34.86
ATOM	1177	CB	ILE	В	980	20.142	32.123	22.676	1.00	27.87
ATOM	1178	CG1	ILE	B	980	20.564	32.314	24.120	1.00	29.18
ATOM	1179	CG2	ILE	В	980	19.778	30.614	22.519	1.00	32.98
ATOM	1180	CD1	ILE	В	980	19.477	32.141	25.157	1.00	26.99
ATOM	1181	N	ALA	В	981	21.425	30.940	19.843	1.00	33.63
ATOM	1182	CA	ALA	В	981	21.100	30.397	18.542	1.00	34.72
ATOM	1183	C	ALA	В	981	20.872	28.883	18.597	1.00	36.94
ATOM	1184	0	ALA	В	981	20.993	28.205	19.630	1.00	36.37
ATOM	1185	CB	ALA	В	981	22.158	30.764	17.532	1.00	32.74
ATOM	1186	N	ASP			20.702	28.316	17.416	1.00	38.89
ATOM	1187	CA	ASP	В	982	20.540	26.898	17.122	1.00	38.46
ATOM	1188	C	ASP	В	982	19.195	26.448	17.713	1.00	37.99
ATOM	1189	0	ASP	В	982	19.092	25.674	18.675	1.00	36.61
ATOM	1190	CB	ASP		982	21.703	26.016	17.541		40.25

17.184

20.728 24.230 16.205 1.00 46.24

1.00 43.41

1191 CG ASP B 982

1192 OD1 ASP B 982

ATOM

ATOM

Title: Method of Identifying Inhibitors of TIE-2 Inventors: Nancy J. Bump et al.

ATOM 1193 OD2 ASP B 982 21.881 23.629 17.877 1.00 42.63
ATOM 1194 N PHE B 983 16.762 26.774 17.503 1.00 41.16
ATOM 1195 C PHE B 983 16.065 25.567 16.890 1.00 42.46
ATOM 1197 O PHE B 983 16.067 25.257 15.664 1.00 43.89
ATOM 1199 C PHE B 983 16.087 25.257 15.664 1.00 43.89
ATOM 1209 C PHE B 983 16.087 25.257 15.664 1.00 43.89
ATOM 1200 C PHE B 983 16.280 29.135 18.179 1.00 39.48
ATOM 1201 CD1 PHE B 983 16.280 29.135 18.179 1.00 39.48
ATOM 1202 CEI PHE B 983 16.280 29.135 18.179 1.00 39.48
ATOM 1202 CEI PHE B 983 16.957 30.289 17.825 1.00 39.97
ATOM 1203 CT2 PHE B 983 16.957 30.289 17.825 1.00 39.97
ATOM 1204 CCI PHE B 983 16.957 30.289 17.835 10.00 39.97
ATOM 1205 CEI PHE B 983 16.957 30.289 12.355 1.00 39.97
ATOM 1204 CCI PHE B 983 16.957 30.289 12.355 1.00 39.97
ATOM 1205 CCI PHE B 983 16.957 30.289 12.0355 1.00 39.97
ATOM 1204 CCI PHE B 983 16.957 30.289 12.0355 1.00 39.97
ATOM 1205 N GLY B 984 15.346 24.852 17.733 1.00 41.51
ATOM 1205 N GLY B 984 15.346 24.852 17.733 1.00 41.51
ATOM 1206 C AG GLY B 984 13.535 23.685 18.500 1.00 40.75
ATOM 1208 C AG GLY B 984 13.535 23.685 18.500 1.00 40.75
ATOM 1209 N LEU B 985 12.781 24.779 18.612 1.00 38.40
ATOM 1210 C LEU B 985 12.781 29.368 18.500 1.00 40.75
ATOM 1210 C LEU B 985 12.781 29.368 18.500 1.00 40.75
ATOM 1210 C LEU B 985 12.781 29.368 18.500 1.00 40.75
ATOM 1211 C LEU B 985 12.781 29.379 10.0 39.83
ATOM 1212 C LEU B 985 12.781 29.379 10.0 39.83
ATOM 1213 CR LEU B 985 12.781 29.379 12.640 1.00 38.29
ATOM 1214 C LEU B 985 12.781 29.379 12.650 1.00 40.75
ATOM 1215 CD1 LEU B 985 12.781 29.379 12.650 1.00 40.75
ATOM 1216 C SEE B 986 9.264 29.392 21.268 1.00 41.75
ATOM 1216 C SEE B 986 9.276 29.273 21.269 1.00 39.62
ATOM 1216 C SEE B 986 9.276 29.273 21.269 1.00 39.62
ATOM 1216 C SEE B 986 9.276 29.273 21.269 1.00 39.62
ATOM 1219 C SEE B 986 9.276 29.292 21.268 1.00 41.75
ATOM 1220 C SEE B 986 9.276 29.292 21.268 1.00 41.75
ATOM 1221 C SEE B 986 9.276 29.292 21.269 1.00 41.75
ATOM 1222 C SEE B 986 9.276 29.292 21.269 1.00 41.75
ATOM 1222 C SEE B 986 9.276 29.292 21.

Docket/App No.: 2079.1037-001

Title: Method of Identifying Inhibitors of TIE-2 Inventors: Nancy J. Bump et al

ATOM	1250	0	GLU	B	9.90	7.134	18.267	26.782	1 00	35.90
ATOM	1251	CB	GLU		990	8.324	17.321	29.615		32.06
ATOM	1252	CG	GLU		990	7.034	16.491	29.549		34.29
ATOM	1253	CD	GLU		990	5.855	16.986	30.361		35.18
ATOM	1254	OE1	GLU		990	4.741	17.354	29.866		31.61
ATOM	1255	OE2	GLU		990	5.907	17.055	31.606		37.46
ATOM	1256	N	VAL		991	9.245	17.586	26.636		28.59
ATOM	1257	CA	VAL		991	9.254	17.187	25.250		27.10
ATOM	1258	C	VAL		991	10.294	16.035	25.123		34.31
ATOM	1259	0	VAL		991	11.499	16.047	25.461		34.01
ATOM	1260	CB	VAL		991	9.566	18.341	24.297		27.78
ATOM	1261	CG1	VAL		991	10.981	18.939	24.577		28.52
ATOM	1262	CG2	VAL		991	9.531	17.878	22.827		26.55
ATOM	1263	N	TYR		992	9.815	15.116	24.284	1.00	33.22
ATOM	1264	CA	TYR		992	10.510	13.950	23.872		35.07
ATOM	1265	c.	TYR		992	11.168	14.196	22.521	1.00	36.09
ATOM	1266	ō	TYR		992	10.453	14.723	21.653		37.35
ATOM	1267	CB	TYR		992	9.504	12.750	23.851	1.00	32.12
ATOM	1268	CG	TYR		992	10.187	11.588	23.154		34.00
MOTA	1269	CD1	TYR		992	10.952	10.664	23.855		35.23
ATOM	1270	CD2	TYR		992	10.065	11.491	21.767		34.41
ATOM	1271	CE1	TYR		992	11.597	9.629	23.205	1.00	
ATOM	1272	CE2	TYR		992	10.706	10.464	21.115		35.88
ATOM	1273	CZ	TYR		992	11.471	9.575	21.830	1.00	
ATOM	1274	OH	TYR		992	12.090	8.582	21.090		41.58
ATOM	1275	N	VAL		993	12.465	13.922	22.409		35.09
ATOM	1276	CA	VAL		993	13.166	14.093	21.148		40.55
ATOM	1277	C	VAL		993	14.192	12.937	21.077		44.20
ATOM	1278	ō	VAL		993	14.924	12.698	22.027		41.10
MOTA	1279	CB	VAL		993	14.027	15.345	20.884		40.80
ATOM	1280	CG1	VAL		993	14.377	15.434	19.397		41.00
ATOM	1281	CG2	VAL	В	993	13.444	16.675	21.308		40.65
ATOM	1282	N	LYS	В	994	14.248	12.280	19.929	1.00	52.91
ATOM	1283	CA	LYS	В	994	15.228	11.218	19.681	1.00	59.67
ATOM	1284	C	LYS	В	994	16.314	11.668	18.722	1.00	63.50
ATOM	1285	0	LYS	В	994	15.968	12.346	17.752	1.00	
ATOM	1286	CB	LYS	В	994	14.452	10.051	19.050	1.00	62.12
ATOM	1287	CG	LYS	В	994	15.258	9.165	18.114	1.00	64.47
ATOM	1288	CD	LYS	В	994	14.523	7.917	17.676	1.00	66.81
ATOM	1289	CE	LYS	В	994	14.741	6.737	18.627	1.00	69.22
ATOM	1290	NZ	LYS	В	994	16.113	6.131	18.446	1.00	70.28
ATOM	1291	N	LYS	В	995	17.568	11.244	18.841	1.00	68.11
ATOM	1292	CA	LYS	В	995	18.698	11.497	17.964	1.00	69.33
ATOM	1293	C	LYS	В	995	19.277	12.900	17.869	1.00	71.04
ATOM	1294	CB	LYS	В	995	18.387	11.058	16.520	1.00	68.75
ATOM	1295	N	THR	В	996	19.210	13.731	18.891	1.00	72.92
ATOM	1296	CA	THR	В	996	19.849	15.039	18.958	1.00	74.27
ATOM	1297	C	THR	В	996	18.897	16.170	18.571	1.00	74.88
ATOM	1298	0	THR		996	17.742	15.867	18.197	1.00	
ATOM	1299	CB	THR	В	996	21.108	15.075	18.098	1.00	74.16
TER										
MOTA	1300	N	LEU	CI	1000	24.923	13.250	19.201	1.00	61.56
ATOM	1301	CA	LEU	CI	1000	24.606	13.627	20.610	1.00	60.45
ATOM	1302	C	LEU	C:	1000	25.273	14.888	21.132	1.00	59.31
ATOM	1303	0			L000	25.926	15.737	20.498	1.00	61.19
ATOM	1304	CB	LEU	C:	L000	25.085	12.439	21.459	1.00	62.33
ATOM	1305	N	PRO	C:	1001	25.106	15.086	22.450	1.00	55.81

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Inventors:

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ATOM

1362 CD1 ILE C1007

25.717 16.238 23.164 1.00 47.68
25.633 15.865 24.622 1.00 42.57
25.066 16.507 25.497 1.00 42.56
25.055 17.514 22.761 1.00 39.19
26.105 13.982 26.180 1.00 36.21
26.526 14.731 27.414 1.00 22.30
27.129 12.774 26.075 1.00 38.41
27.304 12.077 27.400 1.00 36.91
26.315 11.872 25.131 1.00 39.50
27.699 15.354 27.317 1.00 35.59
28.454 16.101 28.310 1.00 35.48 1306 CA PRO C1001 ATOM ATOM 1307 C PRO C1001 PRO C1001 ATOM 1308 0 1309 CB PRO C1001 ATOM VAL C1002 ATOM 1310 N 1311 CA VAL C1002 ATOM ATOM 1312 C VAL C1002 1313 0 VAL C1002 ATOM 1314 CB VAL C1002 ATOM 1315 CG1 VAL C1002 ATOM 1316 CG2 VAL C1002 ATOM 1317 N ARG C1003 ATOM 28.454 16.101 28.310 1.00 34.85 1318 CA ARG C1003 MOTA 27.745 17.378 28.731 1.00 32.80 1319 C ARG C1003 ATOM 28.073 18.089 29.675 1.00 33.09 1320 0 ARG C1003 ATOM ATOM 1321 CB ARG C1003 29.877 16.407 27.775 1.00 35.57 1322 CG ARG C1003 30.017 15.726 26.418 1.00 40.79 ATOM ATOM 1323 CD ARG C1003 31.524 15.638 26.082 1.00 42.74 1324 NE ARG C1003 32.199 15.018 27.219 1.00 46.61 ATOM 1325 CZ ARG C1003 33.482 14.536 26.897 1.00 42.40 ATOM 33.675 14.646 25.606 1.00 44.69 1326 NH1 ARG C1003 ATOM 34.058 13.991 27.899 1.00 41.82 1327 NH2 ARG C1003 ATOM 34.058 13.991 27.899 1.00 41.82 26.753 17.765 27.983 1.00 31.57 25.743 18.792 28.171 1.00 32.26 24.352 18.357 28.588 1.00 33.31 23.571 19.223 29.047 1.00 32.82 25.513 19.633 26.877 1.00 31.61 26.794 20.424 26.649 1.00 29.75 ATOM 1328 N TRP C1004 ATOM 1329 CA TRP C1004 ATOM 1330 C TRP C1004 1331 0 TRP C1004 ATOM ATOM 1332 CB TRP C1004 25.513 19.633 26.877 1.00 31.61 26.75 27.065 21.659 27.174 1.00 33.83 27.885 20.016 25.845 1.00 30.12 28.838 21.058 25.939 1.00 30.12 28.284 18.907 25.81 1.00 31.33 30.114 21.052 25.322 1.00 31.29 29.523 18.911 24.457 1.00 31.63 30.442 19.974 24.537 1.00 31.26 24.039 17.058 28.284 15.799 27.00 30.88 28.284 15.799 27.00 31.29 29.523 18.911 24.457 1.00 31.26 24.039 17.058 28.53 1.00 31.05 22.691 16.644 28.871 1.00 30.92 22.482 16.372 30.342 1.00 31.05 22.595 15.60 30.88 28.53 1.00 31.05 22.505 15.607 26.55 1.00 30.88 22.425 15.401 28.027 1.00 35.78 22.250 15.671 26.542 1.00 35.78 22.331 14.145 25.574 1.00 43.66 20.582 13.671 25.554 1.00 43.66 20.582 13.671 25.554 1.00 30.39 20.980 14.819 32.255 1.00 30.39 20.980 14.243 31.91 1.00 25.95 20.820 14.243 31.91 1.00 25.95 20.820 14.243 31.91 1.00 25.95 20.820 14.243 31.91 1.00 25.95 21.663 14.271 33.445 1.00 23.33 21.99 21.663 14.274 33.351 1.00 23.33 21.99 21.663 14.274 33.351 1.00 23.33 21.99 21.663 24.271 33.351 1.00 32.33 21.99 21.663 24.274 33.351 1.00 32.33 21.99 21.663 24.274 33.351 1.00 32.33 21.99 21.663 24.274 33.351 1.00 32.33 21.99 21.00 24.665 24.274 33.351 1.00 32.33 21.90 24.274 33.351 1.00 32.33 21.90 24.274 33.351 1.00 32.33 21.90 24.274 33.351 1.00 32.33 21.90 24.274 33.351 1.00 32.33 21.90 24.274 1333 CG TRP C1004 ATOM ATOM 1334 CD1 TRP C1004 1335 CD2 TRP C1004 ATOM 1336 NE1 TRP C1004 ATOM ATOM 1337 CE2 TRP C1004 ATOM 1338 CE3 TRP C1004 ATOM 1339 CZ2 TRP C1004 ATOM 1340 CZ3 TRP C1004 1341 CH2 TRP C1004 ATOM 1342 N MET C1005 ATOM 1343 CA MET C1005 ATOM 1344 C MET C1005 ATOM 1345 O MET C1005 ATOM ATOM 1346 CB MET C1005 1347 CG MET C1005 ATOM 1348 SD MET C1005 ATOM 1349 CE MET C1005 ATOM 1350 N ALA C1006 ATOM 1351 CA ALA C1006 1352 C ALA C1006 ATOM ATOM ALA C1006 ATOM 1353 0 1354 CB ALA C1006 ATOM ATOM 1355 N ILE C1007 1356 CA ILE C1007 ATOM 1357 C ILE C1007 19.626 12.254 33.361 1.00 32.33 ATOM 19.539 11.314 32.569 1.00 34.27 1358 O ILE C1007 MOTA 21.316 12.831 35.238 1.00 36.74 ATOM 1359 CB ILE C1007 22.831 12.539 35.418 1.00 40.16 20.535 11.850 36.027 1.00 41.55 ATOM 1360 CG1 ILE C1007 ATOM 1361 CG2 ILE C1007

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23.298 12.738 36.843 1.00 39.53

ATOM	1363	N	CT I	C1008	18.515	12.879	22 560		
ATOM	1364	CA		C1008	17.179	12.879	33.668	1.00 3	
ATOM	1365	C		C1008	17.097	12.390	33.238	1.00 3	
ATOM	1366	Ö		C1008	16.588	11.399	31.725	1.00 3	
ATOM	1367	CB		C1008	16.079	13.201	33.887	1.00 3	2.29
ATOM	1368	CG		C1008	15.861	14.623	33.271		
ATOM	1369	CD		C1008	16.672	15.611	34.070		1.03
MOTA	1370	OE1		C1008	17.610	15.181	34.800	1.00 30	0.62
ATOM	1371	OE2		C1008	16.405	16.824	34.011		3.30
ATOM	1372	N		C1009	17.652	13.397	31.054		3.50
ATOM	1373	CA		C1009	17.665	13.395	29.574		7.96
ATOM	1374	C		C1009	18.551	12.320	29.008		2.36
ATOM	1375	0		C1009	18.258	11.867	27.889		3.49
ATOM	1376	CB		C1009	18.120	14.740	29.001	1.00 2	
ATOM	1377	OG		C1009	17.266	15.856	29.232		9.52
ATOM	1378	N	LEU		19.732	11.948	29.646		0.58
ATOM	1379	CA	LEU	C1010	20.458	10.834	29.043		3.82
ATOM	1380	C	LEU	C1010	19.587	9.543	29.184		1.58
ATOM	1381	0		C1010	19.600	B.647	28.340		3.77
MOTA	1382	CB	LEU		21.835	10.478	29.678		1.39
ATOM	1383	CG	LEU	C1010	22.839	11.659	29.618		1.04
ATOM	1384	CD1		C1010	23.989	11.636	30.582		5.06
ATOM	1385	CD2		C1010	23.324	11.698	28.183		1.32
ATOM	1386	N		C1011	18.894	9.423	30.317		.50
ATOM	1387	CA.		C1011	18.175	8.188	30.585		.53
MOTA	1388	C	ASN		16.867	8.049	29.814		.46
ATOM	1389	0	ASN	C1011	16.521	6.887	29.507	1.00 41	
ATOM	1390	CB	ASN	C1011	17.744	7.990	32.055		7.12
MOTA	1391	CG	ASN	C1011	18.994	7.594	32.849		.42
ATOM	1392	OD1	ASN	C1011	19.913	7.055	32.211		.43
MOTA	1393	ND2	ASN	C1011	18.990	7.876	34.135		7.03
ATOM	1394	N	TYR	C1012	16.144	9.174	29.765		.32
ATOM	1395	CA	TYR	C1012	14.765	9.067	29.205	1.00 33	.71
ATOM	1396	C	TYR	C1012	14.644	9.864	27.929	1.00 37	.07
ATOM	1397	0		C1012	13.431	9.936	27.557	1.00 39	.06
ATOM	1398	ĊВ		C1012	13.779	9.722	30.189	1.00 25	.11
ATOM	1399	CG		C1012	13.979	9.247	31.601	1.00 26	.79
MOTA	1400	CD1		C1012	13.915	10.061	32.704	1.00 28	.02
MOTA	1401	CD2		C1012	14.199	7.868	31.824	1.00 29	.96
ATOM	1402	CEl		C1012	14.075	9.560	33.984	1.00 31	.07
ATOM	1403	CE2		C1012	14.378	7.325	33.070	1.00 30	. 68
ATOM	1404	CZ		C1012	14.310	8.194	34.126	1.00 32	.85
ATOM	1405	OH		C1012	14.494	7.677	35.423	1.00 38	
ATOM	1405	N		C1013	15.568	10.695	27.480	1.00 35	.61
ATOM	1407	CA		C1013	15.244	11.547	26.340	1.00 36	
ATOM	1408	C		C1013	14.080	12.522	26.555	1.00 31	
ATOM ATOM	1409	0		C1013	13.533	12.997	25.558		.49
	1410	CB		C1013	15.021	10.764	25.075		.37
ATOM	1411	og N		C1013	16.000	9.929	24.605	1.00 39	
ATOM	1413			C1014	13.848	12.926	27.798	1.00 34	
ATOM	1414	CA C		C1014	12.887	13.999	28.005		.17
ATOM	1414	0		C1014	13.761	15.212	28.406		. 14
ATOM	1415	CB		C1014 C1014	14.764	15.102	29.061		.92
ATOM	1417			C1014	11.803	13.647	29.007		.91
ATOM	1418	CG2		C1014	10.773	14.771	28.958		. 03
ATOM	1419	N		C1014	11.129	12.316	28.672		.03
			- 41	-1010	17.722	10.3//	27.994	1.00 33	. 31

ATOM	1420	CA	TYR	C1015	13.917	17.662	28.222	1.00 29.96
ATOM	1421	С	TYR	C1015	12,870	18.627	28.713	1.00 32.82
ATOM	1422	ō		C1015	11.635	18.497	28.361	1.00 33.09
ATOM	1423	CB		C1015	14.268	18.208	26.817	1.00 31.34
ATOM	1424	CG		C1015	15.273	17.339	26.106	1.00 32.85
ATOM	1425	CDi		C1015	14.953	16.293	25.270	1.00 33.14
ATOM	1426	CD2		C1015	16.625	17.556	26.338	1.00 33.80
ATOM	1427	CE1		C1015	15.892		24.664	1.00 36.71
ATOM	1427	CE2		C1015		15.497		
	1429	CEZ			17.623	16.791	25.745	1.00 36.63
ATOM				C1015	17.249	15.758	24.895	1.00 36.99
MOTA	1430	OH		C1015	18.233	15.005	24.325	1.00 37.59
ATOM	1431	N		C1016	13.210	19.409	29.691	1.00 29.91
ATOM	1432	CA		C1016	12.342	20.393	30.312	1.00 30.08
MOTA	1433	C		C1016	13.109	21.700	30.459	1.00 33.68
MOTA	1434	0		C1016	14.307	21.752	30.085	1.00 32.46
MOTA	1435	CB		C1016	11.986	19.882	31.717	1.00 31.45
ATOM	1436	OG1		C1016	13.149	19.778	32.540	1.00 31.21
MOTA	1437	CG2	THR	C1016	11.332	18.415	31.720	1.00 29.42
ATOM	1438	N	THR	C1017	12.509	22.699	31.141	1.00 31.49
ATOM	1439	CA	THR	C1017	13.301	23.863	31.536	1.00 32.10
MOTA	1440	C	THR	C1017	14.367	23.447	32.536	1.00 33.86
MOTA	1441	0	THR	C1017	15.480	24.004	32.588	1.00 31.99
ATOM	1442	CB	THR	C1017	12.396	25.033	32.078	1.00 32.15
MOTA	1443	OG1	THR	C1017	11.836	25.456	30.829	1.00 32.91
ATOM	1444	CG2	THR	C1017	13.152	26.192	32.675	1.00 30.94
MOTA	1445	N		C1018	14.062	22.468	33.403	1.00 32.36
ATOM	1446	CA		C1018	15.020	21.997	34.372	1.00 34.23
ATOM	1447	C		C1018	16.208	21.329	33.647	1.00 33.65
ATOM	1448	0		C1018	17.326	21.560	34.163	1.00 32.63
ATOM	1449	CB		C1018	14.563	21.089	35.519	1.00 33.92
ATOM	1450	CG		C1018	13.478	21.750	36.390	1.00 36.18
ATOM	1451	OD1		C1018	13.561	22.943	36.772	1.00 33.93
MOTA	1452	ND2		C1018	12.400	20.983	36.687	1.00 31.82
ATOM	1453	N		C1019	16.007	20.738	32.468	1.00 30.11
ATOM	1454	CA		C1019	17.216	20.101	31.865	1.00 31.68
ATOM	1455	C		C1019	18.016	21.121	31.069	1.00 30.62
ATOM	1456	0		C1019	19.237	21.110	30.787	1.00 35.61
ATOM	1457	CB		C1019	16.668	18.883	31.150	1.00 29.04
ATOM	1458	OG		C1019	16.208	19.177	29.829	1.00 30.35
ATOM	1459	N		C1019	17.331	22.228	30.738	1.00 30.33
ATOM	1460	CA		C1020	17.923	23.429	30.756	1.00 27.36
ATOM	1461	C		C1020		24.034	31.183	1.00 27.36
ATOM	1461	0		C1020	18.880		30.766	
					19.935	24.477		
ATOM	1463	CB		C1020	16.986	24.536	29.714	1.00 28.00
ATOM	1464	CG		C1020	16.480	24.298	28.328	1.00 28.71
ATOM	1465	OD1		C1020	16.969	23.343	27.647	1.00 31.13
ATOM	1466	OD2		C1020	15.583	24.984	27.876	1.00 32.14
MOTA	1467	N		C1021	18.502	24.085	32.455	1.00 26.65
MOTA	1468	CA		C1021	19.328	24.627	33.497	1.00 26.02
ATOM	1469	C		C1021	20.546	23.742	33.781	1.00 27.12
ATOM	1470	0		C1021	21.575	24.333	34.098	1.00 23.97
ATOM	1471	CB		C1021	18.525	24.925	34.779	1.00 27.32
MOTA	1472	CGl		C1021	19.464	25.263	35.929	1.00 25.33
ATOM	1473	CG2	VAL	C1021	17.590	26.138	34.626	1.00 29.37
ATOM	1474	N	TRP	C1022	20.461	22.409	33.671	1.00 25.32
ATOM	1475	CA	TRP	C1022	21.679	21.587	33.868	1.00 23.28
ATOM	1476	C	TRP	C1022	22.664	21.958	32.796	1.00 23.00

ATOM	1477	0	ומיד	C1022	22 025	80 300			
ATOM	1478	CB	TRI		23.835	22.338	32.917		25.36
ATOM	1479	CG	TRE		21.248	20.096	33.625		25.77
ATOM					22.434	19.150	33.646		27.35
	1480	CDI			23.411	18.987	32.695		26.63
ATOM	1481	CD2		C1022	22.685	18.200	34.675		28.39
ATOM	1482	NEI			24.267	18.008	33.079	1.00	29.90
ATOM	1483	CE2			23.840	17.481	34.300	1.00	30.24
ATOM	1484	CE3			22.041	17.867	35.866	1.00	30.30
ATOM	1485	CZ2			24.394	16.485	35.090	1.00	32.33
ATOM	1486	CZ3	TRE	C1022	22.563	16.816	36.624		31.39
ATOM	1487	CH2	TRP	C1022	23.718	16.151	36.243		32.10
ATOM	1488	N	SER	C1023	22.207	21.928	31.529		21.23
ATOM	1489	CA	SER	C1023	23.068	22.354	30.379		22.80
ATOM	1490	C	SER	C1023	23.618	23.745	30.495		27.97
ATOM	1491	0		C1023	24.829	24.031	30.146		23.26
ATOM	1492	CB		C1023	22.108	21.769	29.326		24.28
ATOM	1493	OG		C1023	21.977	22.454	28.131		34.21
ATOM	1494	N		C1024	22.810	24.769	30.968		
ATOM	1495	CA		C1024	23.395	26.101	31.223		24.68
ATOM	1496	C		C1024	24.614	26.101			25.91
ATOM	1497	ō		C1024	25.582		32.155		28.55
ATOM	1498	CB		C1024		26.856	32.091		26.16
ATOM	1499	CG		C1024	22.317	27.041	31.808		23.53
ATOM	1500	CD1			22.904	28.385	32.225		23.34
ATOM	1501	CD2		C1024	22.931	29.409	31.328		21.89
ATOM	1501			C1024	23.322	28.564	33.537		21.62
ATOM		CEL		C1024	33.498	30.640	31.655		24.95
ATOM	1503	CE2		C1024	23.929	29.791	33.858	1.00	25.56
	1504	CZ		C1024	23.957	30.795	32.941	1.00	24.77
ATOM	1505	OH		C1024	24.513	32.006	33.282	1.00	29.84
ATOM	1506	N		C1025	24.559	25.263	33.180	1.00	31.16
ATOM	1507	CA		C1025	25.499	24.901	34.180	1.00	28.63
MOTA	1508	C		C1025	26.812	24.444	33.475	1.00	29.18
ATOM	1509	0	GLY	C1025	27.826	24.973	33.911	1.00	25.38
MOTA	1510	N	VAL	C1026	26.724	23.628	32.431	1.00	
MOTA	1511	CA	VAL	C1026	27.848	23.171	31.665	1.00	30.49
MOTA	1512	C	VAL	C1026	28.404	24.335	30.867	1.00	
MCTA	1513	0	VAL	C1026	29.622	24.566	30.796		31.75
ATOM	1514	CB	VAL	C1026	27.598	21.959	30.748	1.00	
MOTA	1515	CG1	VAL	C1026	28.867	21.451	30.040		26.68
ATOM	1516	CG2	VAL	C1026	26.960	20.808	31.527		28.00
ATOM	1517	N	LEU	C1027	27.539	25.107	30.208		29.76
ATOM	1518	CA	LEU	C1027	27.925	26.331	29.524		27.25
ATOM	1519	C		C1027	28.729	27.263	30.410		25.12
MOTA	1520	0		C1027	29.764	27.833	30.030		27.00
ATOM	1521	CB		C1027	26.664	27.044	28.959		27.55
ATOM	1522	CG		C1027	26.904	28.561	28.667		27.68
ATOM	1523	CD1		C1027	27.658	28.914	27.434		
MOTA	1524	CD2		C1027	25.485	29.174	28.511		28.77
ATOM	1525	N		C1028	28.311	27.500		1.00	29.96
ATOM	1526	CA		C1028	28.311		31.665		27.12
ATOM	1527	C		C1028		28.386	32.576	1.00	26.05
ATOM	1528	0		C1028	30.399	27.853	32.836	1.00	28.29
ATOM	1529	CB			31.296	28.666	32.888	1.00	27.74
ATOM	1530	CG		C1028	28.123	28.576	33.809	1.00	24.95
ATOM	1531	CD1		C1028	28.601	29.349	34.990	1.00	
ATOM	1531	CD1		C1028	28.932	30.805	34.567	1.00	26.51
ATOM	1533	N		C1028	27.771	29.411	36.264		23.62
		7.0	LECT	C1029	30.569	26.514	32.998	1.00	27.52

ATOM	1534	CA	ם קיד	C1029	31.811	25.818	33.200	1.00 25.28
ATOM	1535	C		C1029	32.677	26.052	31.992	1.00 24.21
ATOM	1536	0		C1029	33.809	26.411	32.199	1.00 28.34
ATOM	1537	CB		C1029	31 604	24.291	33.488	1.00 25.54
ATOM	1538	CG		C1029	32.875	23.609	33.400	1.00 25.52
ATOM	1539	CD1	TRP	C1029	33.316	23.467	35.159	1.00 23.77
ATOM	1540	CD2		C1029	33.901	23.125	33.013	1.00 25.22
ATOM	1541	NEl	TRP		34.566	22.870	35.125	1.00 28.07
ATOM	1542	CE2	TRP	C1029	34.922	22.645	33.819	1.00 27.51
MOTA	1543	CE3	TRP	C1029	34.013	23.005	31.620	1.00 27.28
ATOM	1544	CZ2	TRP	C1029	36.095	21.998	33.349	1.00 30.61
ATOM	1545	CZ3		C1029	35.169	22.378	31.126	1.00 30.99
ATOM	1546	CH2	TRP	C1029	36.195	21.931	31.972	1.00 29.91
ATOM	1547	N	GLU	C1030	32.196	26.006	30.773	1.00 22.75
ATOM	154B	CA	GLU	C1030	32.865	26.380	29.590	1.00 24.64
ATOM	1549	C	GLU	C1030	33.291	27.882	29.553	1.00 23.46
ATOM	1550	0	GLU	C1030	34.433	28.114	29.047	1.00 23.61
ATOM	1551	CB	GLU	C1030	32.036	26.144	28.339	1.00 22.23
ATOM	1552	CG	GLU	C1030	31.853	24.671	28.076	1.00 27.85
ATOM	1553	CD		C1030	30.969	24.399	26.881	1.00 33.40
ATOM	1554	OE1		C1030	29.767	24.531	27.111	1.00 33.08
ATOM	1555	OE2		C1030	31.477	24.088	25.792	1.00 37.59
ATOM	1556	N		C1031	32.413	28.784	30.027	1.00 20.93
ATOM	1557	CA		C1031	32.888	30.190	29.987	1.00 23.32
ATOM	1558	C		C1031	34.099	30.417	30.881	1.00 24.20
ATOM	1559	0		C1031	35.125	31.060	30.547	1.00 24.20
ATOM	1560	СВ		C1031	31.720	31.156		
ATOM	1561	CG1		C1031	30.622	31.156	30.365	1.00 22.53
ATOM	1562			C1031				
	1563	CG2		C1031	32.262	32.584	30.449	1.00 25.77
ATOM		CD1			29.254	31.567	29.766	1.00 24.02
ATOM	1564	N		C1032	34.002	30.128	32.180	1.00 23.96
ATOM	1565	CA		C1032	34.923	30.263	33.255	1.00 28.42
ATOM	1566	C		C1032	36.251	29.547	32.943	1.00 31.87
ATOM	1567	0		C1032	37.324	30.118	33.157	1.00 31.88
MOTA	1568	CB		C1032	34.229	29.636	34.479	1.00 31.74
ATOM	1569			C1032	35.145	28.990	35.490	1.00 35.56
ATOM	1570	CG2		C1032	33.241	30.562	35.210	1.00 29.88
ATOM	1571	Ŋ		C1033	36.236	28.433	32.262	1.00 29.60
ATOM	1572	CA		C1033	37.352	27.612	31.846	1.00 29.62
ATOM	1573	C		C1033	37.900	28.101	30.520	1.00 30.68
ATOM	1574	0	SER	C1033	38.900	27.598	30.046	1.00 30.21
ATOM	1575	CB	SER	C1033	36.909	26.139	31.703	1.00 30.12
ATOM	1576	OG	SER	C1033	36.408	25.725	30.430	1.00 30.39
ATOM	1577	И	LEU	C1034	37.291	29.100	29.905	1.00 28.42
ATOM	1578	CA	LEU	C1034	37.787	29.635	28.638	1.00 31.98
ATOM	1579	C	LEU	C1034	37.753	28.432	27.688	1.00 32.37
ATOM	1580	0	LEU	C1034	38.731	27.936	27.147	1.00 39.15
ATOM	1581	CB	LEU	C1034	39.205	30.261	28.704	1.00 29.58
ATOM	1582	CG	LEU	C1034	39.466	31.409	29.630	1.00 28.94
ATOM	1583	CD1		C1034	40.895	31.922	29.656	1.00 30.58
ATOM	1584	CD2		C1034	38.617	32.636	29.209	1.00 26.58
ATOM	1585	И		C1035	36.530	27.864	27.544	1.00 28.98
ATOM	1586	CA		C1035	36.357	26.754	26.647	1.00 24.56
ATOM	1587	C		C1035	37.171	25.481	26.790	1.00 20.81
ATOM	1588	0		C1035	37.321	24.796	25.771	1.00 21.90
ATOM	1589	N		C1036	37.326	24.968	27.997	1.00 21.82
ATOM	1590	CA		C1036	37.834	23.629	28.239	1.00 25.47
				-1000	51.034	20.029	20.225	2.00 20.47

MOTA	1591	С	GLY	C1036	36.727	22.590	27.923	1.00 28.57
ATOM	1592	0	GLY	C1036	35.562	22.944	28.062	1.00 33.09
MOTA	1593	N	THR	C1037	37.098	21.424	27.446	1.00 31.18
ATOM	1594	CA	THR	C1037	36.071	20.402	27.101	1.00 31.40
ATOM	1595	C	THR	C1037	35.671	19.771	28.411	1.00 29.08
ATOM	1596	0	THR	C1037	36.402	19.322	29.267	1.00 28.43
ATOM	1597	CB	THR	C1037	36.849	19.362	26.248	1.00 35.25
MOTA	1598	OG1	THR	C1037	37.143	19.856	24.934	1.00 34.77
ATOM	1599	CG2	THR	C1037	36.056	18.071	26.103	1.00 39.81
ATOM	1600	N	PRO	C1038	34.318	19.849	28.643	1.00 28.79
ATOM	1601	CA		C1038	33.748	19.251	29.832	1.00 29.26
ATOM	1602	C	PRO	C1038	34.121	17.764	29.891	1.00 30.33
ATOM	1603	0		C1038	34.045	17.064	28.877	1.00 30.70
	. 1604	CB		C1038	32.262	19.472	29.632	1.00 29.45
ATOM	1605	CG		C1038	32.146	20.595	28.674	1.00 26.90
ATOM	1606	CD		C1038	33.290	20.373	27.726	1.00 26.24
MCTA	1607	N		C1039	34.507	17.239	31.019	1.00 27.10
ATOM	1608	CA		C1039	34.831	15.865	31.319	1.00 31.51
ATOM	1609	С		C1039	35.958	15.322	30.451	1.00 33.48
ATOM	1610	0		C1039	36.068	14.191	29.947	1.00 32.47
ATOM	1611	CB		C1039	33.580	14.968	31.246	1.00 29.03
ATOM	1612	CG		C1039	32.355	15.453	31.980	1.00 28.35
ATOM	1613			C1039	31.290	15.997	31.247	1.00 27.58
ATOM	1614			C1039	32.220	15.368	33.364	1.00 26.44
ATOM	1615	CE1		C1039	30.142	16.486	31.827	1.00 23.25
ATOM	1616	CE2		C1039	31.053	15.846	33.969	1.00 25.69
MOTA	1617	CZ		C1039	30.031	16.398	33.196	1.00 25.31
MOTA	1618	OH		C1039	28.870	16.776	33.851	1.00 28.82
ATOM	1619	N		C1040	3€.877	16.276	30.243	1.00 37.16
ATOM	1620	CA		C1040	38.045	16.095	29.389	1.00 38.31
ATOM	1621	C		C1040	38.733	14.821	29.848	1.00 36.75
ATOM ATOM	1622 1623	0		C1040	38.962	14.593	31.042	1.00 33.37
ATOM	1624	CB		C1040	38.886	17.360	29.511	1.00 41.12
ATOM	1625	SG N		C1040	40.570	17.157	28.904	1.00 52.08
ATOM	1626	CA		C1041	38.916	13.899	28.920	1.00 38.90
ATOM	1627	C		C1041 C1041	39.550	12.613	29.230	1.00 43.75
ATOM	1628	0		C1041	38.531	11.489	29.459	1.00 46.25
ATOM	1629	N		C1041	38.940 37.288	10.313	29.384	1.00 45.71
ATOM	1630	CA		C1042	36.267	11.831	29.785	1.00 46.22
ATOM	1631	C		C1042	35.471	10.832	30.078	1.00 47.06
ATOM	1632	Õ		C1042	35.257	11.143	28.874	1.00 47.05
ATOM	1633	CB		C1042	35.281	11.343	31.119	1.00 47.49 1.00 46.72
ATOM	1634	CG		C1042	35.944	11.545	32.445	
ATOM	1635	SD		C1042	34.712	11.819	33.734	1.00 48.06 1.00 51.59
ATOM	1636	CE		C1042	33.816	10.274	33.378	1.00 51.12
ATOM	1637	N		C1043	35.143	9.097	28.852	1.00 48.58
ATOM	1638	CA		C1043	34.359	8.548	27.745	1.00 50.37
ATOM	1639	C		C1043	32.867	8.824	27.743	1.00 49.20
ATOM	1640	ō		C1043	32.469	8.990	29.090	1.00 48.53
ATOM	1641	CB		C1043	34.541	7.022	27.715	1.00 49.50
ATOM	1642	OG1		C1043	33.825	6.420	28.780	1.00 49.50
ATOM	1643	CG2		C1043	36.053	6.740	27.911	1.00 48.66
MOTA	1644	N		C1044	32.090	8.784	26.869	1.00 52.39
ATOM	1645	CA		C1044	30.591	8.992	27.031	1.00 54.39
ATOM	1646	C		C1044	30.054	7.913	27.964	1.00 55.34
ATOM	1647	0	CYS	C1044	29.373	8.230	28.952	1.00 56.27

ATOM	1648	CB	CVC	C1044	29.890	9.166	25.699	1.00 54.86
ATOM	1649	SG		C1044	30.275	10.658	24.717	1.00 54.85
ATOM	1650	N		C1044	30.546	6.684	27.883	1.00 53.74
ATOM	1651	CA		C1045	30.276	5.533		
							28.691	1.00 53.52
ATOM	1652	C		C1045	30.319	5.704	30.200	1.00 52.95
ATOM	1653	0		C1045	29.467	5.296	31.022	1.00 52.64
ATOM	1654	CB		C1045	31.379	4.491	28.321	1.00 54.24
ATOM	1655	N		C1046	31.440	6.277	30.650	1.00 50.91
ATOM	1656	CA		C1046	31.637	6.589	32.076	1.00 48.71
ATOM	1657	С		C1046	30.675	7.673	32.539	1.00 46.60
ATOM	1658			C1046	30.237	7.666	33.717	1.00 44.26
ATOM	1659	CB		C1046	33.085	7.002	32.314	1.00 49.93
ATOM	1660	CG	GLU	C1046	34.115	6.109	31.628	1.00 53.13
ATOM	1661	CD	GLU	C1046	35.513	6.735	31.729	1.00 54.82
ATOM	1662	OE1	GLU	C1046	36.134	6.539	32.795	1.00 54.82
ATOM	1663	OE2	GLU	C1046	35.963	7.416	30.783	1.00 55.96
ATOM	1664	N	LEU	C1047	30.268	8.586	31.614	1.00 45.34
ATOM	1665	CA	LEU	C1047	29.331	9.632	32.066	1.00 44.07
MOTA	1666	С	LEU	C1047	27.983	9.017	32.439	1.00 42.99
ATOM	1667	0	LEU	C1047	27.530	9.215	33.576	1.00 42.01
ATOM	1668	CB	LEU	C1047	29.181	10.815	31.111	1.00 45.07
ATOM	1669	CG		C1047	30.430	11.706	30.918	1.00 44.08
ATOM	1670	CD1		C1047	30.038	12.921	30.115	1.00 45.50
ATOM	1671	CD2		C1047	31.071	12.058	32.245	1.00 42.85
ATOM	1672	N		C1048	27.409	8.182	31.588	1.00 43.22
ATOM	1673	CA		C1048	26.213	7.392	31.910	1.00 44.38
ATOM	1674	C		C1048	26.397	6.646	33.245	1.00 44.87
ATOM	1675	0		C1048	25.486	6.717	34.085	1.00 44.87
ATOM	1676	CB		C1048	25.905	6.343		
ATOM	1677	CG		C1048	25.256	6.871	30.853	1.00 44.96
ATOM	1678	CD1		C1048	26.033	7.330	28.545	1.00 47.81
ATOM	1679			C1048				
		CD2			23.852	6.898	29.482	1.00 48.40
ATOM	1680	CE1		C1048	25.436	7.802	27.387	1.00 47.27
ATOM	1681	CE2		C1048	23.246	7.366	28.324	1.00 48.08
ATOM	1682	CZ		C1048	24.075	7.815	27.294	1.00 48.94
ATOM	1683	OH		C1048	23.413	8.274	26.168	1.00 49.94
ATOM	1684	N		C1049	27.591	6.069	33.477	1.00 42.94
ATOM	1685	CA		C1049	27.749	5.400	34.754	1.00 45.35
ATOM	1686	С		C1049	28.155	6.333	35.873	1.00 44.67
ATOM	1687	0		C1049	27.588	6.137	36.975	1.00 45.76
ATOM	1688	CB		C1049	28.683	4.171	34.686	1.00 47.30
ATOM	1689	CG		C1049	30.158	4.453	34.837	1.00 49.28
ATOM	1690	CD		C1049	31.072	3.245	35.050	1.00 50.85
MOTA	1691	OE1		C1049	31.702	2.810	34.042	1.00 51.60
ATOM	1692	OE2	GLU	C1049	31.179	2.748	36.200	1.00 49.78
ATOM	1693	N	LYS	C1050	29.038	7.320	35.685	1.00 45.45
ATOM	1694	CA	LYS	C1050	29.387	8.148	36.861	1.00 46.05
ATOM	1695	C	LYS	C1050	28.404	9.253	37.175	1.00 44.76
MOTA	1696	0	LYS	C1050	28.099	9.497	38.375	1.00 44.16
ATOM	1697	CB	LYS	C1050	30.814	8.668	36.707	1.00 49.41
ATOM	1698	CG	LYS	C1050	31.798	7.565	36.380	1.00 52.04
ATOM	1699	CD		C1050	33.285	7.938	36.456	1.00 54.77
ATOM	1700	CE		C1050	34.086	6.629	36.533	1.00 56.01
ATOM	1701	NZ	LYS	C1050	35.565	6.819	36.433	1.00 58.90
ATOM	1702	N		C1051	27.733	9.813	36.163	1.00 41.92
ATOM	1703	CA		C1051	26.746	10.866	36.552	1.00 43.18
ATOM	1704	C		C1051	25.759	10.435	37.607	1.00 43.10
		-		-1001	2333	.0.433	37.007	2.00 23.33

~ FIG. 5DD

1705 O LEU C1051

1706 CB LEU C1051

1707 CG LEU C1051

1708 CD1 LEU C1051

MOTA

ATOM

ATOM

MOTA

ATOM ATOM MOTA

ATOM

1761 N GLU C1058

25.582 11.062 38.662 1.00 43.64

26.145 11.496 35.307 1.00 43.49 27.096 12.382 34.480 1.00 42.95 26.331 12.985 33.326 1.00 43.01

	MCTA	1709	CD2	LEU	C1051	27.702	13.468	35.366	1.00 43.66
	MOTA	1710	N	PRO	C1052	25.084	9.288	37.475	1.00 45.02
	ATOM	1711	CA	PRO	C1052	24.140	8.817	38.470	1.00 45.84
	ATOM	1712	C	PRO	C1052	24.736	8.635	39.839	1.00 47.07
	ATOM	1713	0	PRO	C1052	24.088	8.826	40.880	1 00 48.20
	ATOM	1714	CB	PRO	C1052	23.559	7.544	37.854	1.00 45.47
	ATOM	1715	CG	PRO	C1052	23.652	7.799	36.384	1.00 44.83
	MCTA	1716	CD	PRO	C1052	25.013	8.487	36.242	1.00 45.28
	ATOM	1717	N	GLN	C1053	26.006	8.296	40.007	1.00 50.49
	ATOM	1718	CA	GLN	C1053	26.594	8.130	41.331	1.00 52.45
	ATOM	1719	C	GLN	C1053	26.921	9.462	41.976	1.00 51.74
	ATOM	1720	0	GLN	C1053	27.231	9.442	43.175	1.00 51.45
	ATOM	1721	CB	GLN	C1053	27.798	7.199	41.221	1.00 55.75
	ATOM	1722	CG	GLN	C1053	27.411	5.794	40.768	1.00 61.04
	ATOM	1723	CD		C1053	26.526	5.041	41.743	1.00 64.91
1.1	ATOM	1724	OEl	GLN	C1053	26.851	4.904	42.948	1.00 66.92
+0	ATOM	1725	NE2	GLN	C1053	25.370	4.528	41.286	1.00 65.52
(4)	ATOM	1726	N		C1054	26.801	10.624	41.320	1.00 49.79
p-de	ATOM	1727	CA		C1054	27.061	11.874		1.00 46.62
7,51	ATOM	1728	C		C1054	28.276	12.597	41.495	1.00 44.62
1,43	ATOM	1729	0		C1054	28.683	13.662	41.920	1.00 43.65
10.00	ATOM	1730	N		C1055	28.917	12.051	40.482	1.00 45.48
fadi.	ATOM	1731	CA		C1055	30.099	12.698	39.937	1.00 45.51
	ATOM	1732	C		C1055	29.685	13.995	39.214	1.00 44.95
# #75	ATOM	1733	0		C1055	28.622	13.976	38.583	1.00 46.39
Cal	ATOM	1734	CB		C1055	30.767	11.776	38.932	1.00 45.73
11.5	ATOM	1735	CG		C1055	32.055	12.414	38.433	1.00 48.52
TU	ATOM	1736			C1055	33.235	12.302	39.143	1.00 48.82
111	ATOM	1737			C1055	32.045	13.129	37.234	1.00 48.37
2000	ATOM	1738			C1055	34.401	12.898	38.658	1.00 48.87
broke	ATOM	1739			C1055	33.178	13.723	36.737	1.00 47.42
	ATOM	1740	CZ		C1055	34.354	13.582	37.459	1.00 49.27
	ATOM	1741	OH		C1055	35.488	14.170	36.952	1.00 48.77
	ATOM	1742	N		C1056	30.485	15.051	39.252	1.00 40.28
	MOTA	1743	CA		C1056	30.189		38.566	1.00 38.71
	ATOM	1744	C		C1056	31.481	17.012	38.176	1.00 39.85
	ATOM	1745	ō		C1056	32.472	16.797	38.879	1.00 42.11
	ATOM	1746	CB	ARG	C1056	29.407		39.408	1.00 38.04
	ATOM	1747	CG		C1056	27.996		39.890	1.00 37.78
	MCTA	1748	CD	ARG	C1056	27.022	16.584	38.810	1.00 34.37
	ATOM	1749	NE		C1056	25.677		39.370	1.00 32.75
	ATOM	1750	CZ		C1056	25.172	15.135	39.461	1.00 34.13
	ATOM	1751			C1056	23.934		39.951	1.00 33.89
	ATOM	1752			C1056	25.884			
	ATOM	1753	N		C1057	31.450			
	ATOM	1754	CA		C1057	32.615			
	ATOM	1755	C		C1057	33.280			
	ATOM	1756	0		C1057	32.759		39.007	
	ATOM	1757	CB		C1057	32.223			
	7.77034				01057				1 00 40 26

34,597 19,231 37,962 1,00 38,47

1756 CG LEU C1057 21.870 19.236 34.492 1.00 40.26 1759 CD1 LEU C1057 31.190 20.384 33.790 1.00 41.53 1760 CD2 LEU C1057 33.089 18.719 33.746 1.00 44.03

ATOM	1762	CA							
ATOM	1763	CA		C1058	35.494	19.715	39.003		40.99
ATOM	1764	0		C1058	35.655	21.237	38.941		37.60
ATOM	1765	CB		C1058	35.665	21.759	37.841		37.18
ATOM	1766	CG		C1058	36.808	18.952	38.778		43.93
ATOM	1767	CD	GLU		37.256	18.728	37.367		49.34
ATOM	1768				36.540	18.005	36.265		51.18
ATOM	1769	OE1		C1058	36.581	18.538	35.121		50.19
ATOM	1770	N	LYS		35 931	16.902	36.361		52.82
ATOM	1771	CA	LYS		35.708	21.975	49.005		35.88
ATOM	1771	CA	LYS		35.948	23.424	39.950		40.12
ATOM	1773	0			37.345	23.831	39.473		41.54
ATOM	1774	CB		C1059	38.332	23.431	40.095		41.88
ATOM	1775			C1059	35.946	23.896	41.417		39.21
		CG		C1059	35.984	25.413	41.569		41.97
ATOM	1776	CD		C1059	35.953	25.810	43.048		43.62
ATOM	1777	CE		C1059	37.349	25.786	43.641		43.92
ATOM	1778	NZ		C1059	38.192	26.906	43.099	1.00	44.39
ATOM	1779	N		C1060	37.498	24.651	38.439	1.00	41.99
ATOM	1780	CA		C1060	38.795	25.166	38.040	1.00	42.27
ATOM	1781	С		C1060	39.441	25.920	39.186	1.00	42.45
ATOM	1782	0		C1060	38.840	26.618	39.996	1.00	40.76
ATOM	1783	CB		C1060	38.529	26.115	36.894	1.00	43.06
ATOM	1784	CG		C1060	37.145	25.765	36.416	1.00	41.60
ATOM	1785	CD		C1060	36.408	25.170	37.589	1.00	41.74
ATOM	1786	N	LEU	C1061	40.773	25.843	39.287	1.00	44.11
ATOM	1787	CA	LEU	C1061	41.557	26.440	40.325	1.00	44.84
ATOM	1788	C	LEU	C1061	41.416	27.941	40.443	1.00	44.71
ATOM	1789	0	LEU	C1061	41.441	28.470	41.567	1.00	45.26
MOTA	1790	CB		C1061	43.036	26.089	40.055		48.79
ATOM	1791	CG		C1061	43.314	24.624	40.459	1.00	52.11
ATOM	1792	CD1		C1061	44.673	24.204	39.897	1.00	53.08
ATOM	1793	CD2		C1061	43.288	24.512	41.984	1.00	52.05
ATOM	1794	N		C1062	41.247	28.623	39.321	1.00	44.44
ATOM	1795	CA	ASN	C1062	41.112	30.085	39.327	1.00	44.45
ATOM	1796	C	ASN	C1062	39.661	30.582	39.363	1.00	44.24
ATOM	1797	0	ASN	C1062	39.394	31.757	39.073	1.00	42.70
ATOM	1798	CB	ASN	C1062	41.811	30.536	38.059	1.00	47.14
ATOM	1799	CG	ASN	C1062	41.018	30.280	36.799	1.00	50.71
MOTA	1800	OD1	ASN	C1062	40.297	29.260	36.680	1.00	55.26
ATOM	1801	ND2	ASN	C1062	41.160	31.208	35.873	1.00	49.84
ATOM	1802	M	CYS	C1063	38.727	29.727	39.787		40.21
ATOM	1803	CA	CYS	C1063	37.312	30.006	39.917		39.16
MOTA	1804	C	CYS	C1063	36.922	30.226	41.375		40.26
MOTA	1805	0	CYS	C1063	37.149	29.298	42.177		38.11
ATOM	1806	CB	CYS	C1063	36.476	28.796	39.430		36.02
ATOM	1807	SG	CYS	C1063	34.684	29.162	39.283		36.25
MOTA	1808	N	ASP	C1064	36.179	31.287	41.675		39.98
ATOM	1809	CA	ASP	C1064	35.704	31.514	43.034		42.23
ATOM	1810	C	ASP	C1064	34.623	30.474	43.367		43.63
ATOM	1811	0	ASP	C1064	33.885	29.998	42.516		42.13
ATOM	1812	CB	ASP	C1064	35.166	32.915	43.277		44.24
ATOM	1813	CG	ASP	C1064	34.744	33.348	44.660		47.38
ATOM	1814	ODl	ASP	C1064	35.591	34.016	45.335		49.14
ATOM	1815	OD2		C1064	33.594	33.165	45.169		46.30
ATOM	1816	N		C1065	34.571	30.128	44.646		44.20
ATOM	1817	CA		C1065	33.681	29.213	45.285		46.41
ATOM	1818	C		C1065	32.214	29.629	45.059		46.09

		_		04055	31.383	28.772	44.807	1.00 45.90
MOTA	1819	0		C1065	31.383	29.111	44.807	1.00 49.84
ATOM	1820	CB		C1065				
ATOM	1821	CG		C1065	34.972	28.020	47.179	1.00 54.04
ATOM	1822	OD1		C1065	35.370	27.139	46.384	
ATOM	1823	OD2		C1065	35.412	27.941	48.364	1.00 56.55
ATOM	1824	N		C1066	31.932	30.931	44.991	1.00 46.33
MOTA	1825	CA		C1066	30.585	31.364	44.699	1.00 46.37
ATOM	1826	C		C1066	30 162	30.946	43.279	1.00 43.58
MOTA	1827	0		C1066	28.974	30.622	43.161	1.00 40.53
MCTA	1828	CB		C1066	30 362	32.870	44.901	1.00 47.78
ATOM	1829	CG		C1066	30.464	33.371	46.327	1.00 51.27
ATOM	1830	CD	GLU	C1066	30.147	34.853	46.483	1.00 54.46
MOTA	1831	OE1	GLU	C1066	30.977	35.632	47.023	1.00 56.49
ATOM	1832	OE2	GLU	C1066	29.039	35.278	46.075	1.00 54.91
MOTA	1833	7.1	VAL	C1067	31.031	31.026	42.267	1.00 40.02
ATOM	1834	CA	VAL	C1067	30.592	30.670	40.914	1.00 38.39
ATOM	1835	C	VAL	C1067	30.361	29.166	40.750	1.00 38.56
ATOM	1836	0	VAL	C1067	29.492	28.741	39.975	1.00 35.01
ATOM	1837	CB	VAL	C1067	31.561	31.094	39.797	1.00 37.83
MOTA	1838	CGl	VAL	C1067	31.071	30.760	38.416	1.00 34.84
ATOM	1839	CG2	VAL	C1067	31.809	32.609	39.878	1.00 39.35
ATOM	1840	N	TYR	C1068	31.258	28.419	41.393	1.00 37.89
ATOM	1841	CA	TYR	C1068	31.203	26.969	41.346	1.00 38.97
ATOM	1842	C	TYR	C1068	29.924	26.510	42.044	1.00 40.70
MOTA	1843	0	TYR	C1068	29.265	25.613	41.492	1.00 38.63
ATOM	1844	CB	TYR	C1068	32.437	26.278	41.913	1.00 37.20
ATOM	1845	CG	TYR	C1068	32.470	24.770	41.798	1.00 35.05
ATOM	1846	CD1	TYR	C1068	32.535	24.158	40.556	1.00 34.59
ATOM	1847	CD2	TYR	C1068	32.431	23.934	42.903	1.00 35.51
ATOM	1848	CE1	TYR	C1068	32.536	22.785	40.405	1.00 33.51
ATOM	1849	CE2	TYR	C1068	32.456	22.549	42.800	1.00 33.38
ATOM	1850	CZ	TYR	C1068	32.540	22.006	41.540	1.00 33.70
ATOM	1851	OH	TYR	C1068	32.545	20.637	41.342	1.00 37.05
ATOM	1852	N	ASP	C1069	29.573	27.177	43.159	1.00 42.06
ATOM	1853	CA	ASP	C1069	28.316	26.862	43.806	1.00 42.68
ATOM	1854	C	ASP	C3069	27.124	27.069	42.869	1.00 40.99
ATOM	1855	0	ASP	C1069	26.233	26.193	42.884	1.00 40.08
ATOM	1856	CB	ASP	C1069	28.116	27.676	45.094	1.00 47.98
ATOM	1857	CG	ASP	C1069	28.983	27.092	46.212	1.00 53.70
ATOM	1858	OD1	ASP	C1069	29.487	25.940	46.045	1.00 55.80
MOTA	1859	OD2		C1069	29.161	27.786	47.254	1.00 55.99
ATOM	1860	N		C1070	27.080	28.150	42.087	1.00 36.81
ATOM	1861	CA	LEU	C1070	25.977	28.308	41.140	1.00 36.03
ATOM	1862	C	LEU	C1070	25.905	27.172	40.123	1.00 34.83
ATOM	1863	0	LEU	C1070	24.833	26.703	39.743	1.00 32.57
ATOM	1864	CB	LEU	C1070	26.131	29.666	40.472	1.00 33.68
ATOM	1865	CG	LEU	C1070	25.095	30.113	39.458	1.00 35.12
ATOM	1866			C1070	23.674	29.955	40.003	1.00 34.71
ATOM	1867			C1070	25.391	31.582	39.084	1.00 34.63
MCTA	1868	N		C1071	27.036	26.703	39.602	1.00 36.71
ATOM	1869	CA		C1071	27.131	25.568	38.706	1.00 37.17
MOTA	1870	C		C1071	26.555	24.302	39.372	1.00 36.93
MOTA	1871	0		C1071	25.808	23.574	38.735	1.00 36.82
ATOM	1872	CB		C1071	28.569	25.145	38.294	1.00 35.35
ATOM	1873	CG	MET		29.354	26.145	37.465	1.00 35.64
ATOM	1874	SD		C1071	31.096	25.645	37.207	1.00 32.11
ATOM	1875	CE	MET	C1071	31.839	27.209	36.753	1.00 34.27

ATOM	1876	N	n n c	C1072	26.959	22 042		3 00 05 83
ATOM	1877	CA		C1072	26.550	23.943	40.580	1.00 36.71
MOTA	1878	C	ARG		25.039	22.687	41.323	1.00 37.27
ATOM	1879	0	ARG		24.384			1.00 36.15
ATOM	1880	CB	ARG	C1072	27.272	21.638 22.810	41.587	1.00 37.31
ATOM	1881	CG		C1072	28.773	22.514	42.713	1.00 39.01
ATOM	1882	CD	ARG		29.110	21.260	41.887	1.00 38.84
ATOM	1883	NE	ARG					1.00 40.99
ATOM	1884	CZ			28.618	20.088	42.608	1.00 45.98
ATOM	1885	NH1		C1072	29.217	19.090	43.239	1.00 46.52
					30.532	18.968	43.255	1.00 44.60
ATOM	1886	NH2		C1072	28.428	18.173	43.842	1.00 46.54
ATOM	1887	N		C1073	24.427	23.832	41.775	1.00 36.36
ATOM	1888	CA		C1073	22.986	24.010	41.934	1.00 36.84
ATOM	1889	C		C1073	22.289	23.680	40.612	1.00 35.17
MOTA	1890	0		C1073	21.240	23.043	40.616	1.00 36.12
ATOM	1891	CB		C1073	22.690	25.436	42.324	1.00 40.62
MOTA	1892	CG		C1073	22.926	25.928	43.737	1.00 44.26
ATOM	1893	CD		C1073	22.601	27.425	43.797	1.00 48.97
ATOM	1894	OEl		C1073	22.895	28.160	44.746	1.00 50.88
ATOM	1895	NE2		C1073	21.954	27.977	42.770	1.00 50.58
ATOM	1896	M	CYS	C1074	22.888	23.925	39.463	1.00 34.02
ATOM	1897	CA	CYS	C1074	22.346	23.554	38.175	1.00 33.44
ATOM	1898	C	CYS	C1074	22.300	22.048	37.953	1.00 32.85
ATOM	1899	0	CYS	C1074	21.595	21.573	37.050	1.00 28.15
MOTA	1900	CB	CYS	C1074	23.165	24.222	37.052	1.00 32.80
ATOM	1901	SG	CYS	C1074	22.926	26.054	36.945	1.00 29.54
ATOM	1902	N	TRP	C1075	23.155	21.300	38.651	1.00 34.38
ATOM	1903	CA	TRP	C1075	23.323	19.869	38.394	1.00 36.36
ATOM	1904	C	TRP	C1075	22.772	19.008	39.538	1.00 37.35
ATOM	1905	0	TRP	C1075	23.378	17.961	39.809	1.00 36.14
ATOM	1906	CB	TRP	C1075	24.797	19.516	38.184	1.00 31.61
ATOM	1907	CG	TRP	C1075	25.554	20.319	37.170	1.00 32.01
ATOM	1908	CD1	TRP	C1075	25.035	20.735	35.945	1.00 30.72
ATOM	1909	CD2	TRP	C1075	26.905	20.792	37.215	1.00 27.71
ATOM	1910	NE1	TRP	C1075	26.028	21.458	35.263	1.00 27.75
ATOM	1911	CE2		C1075	27.165	21 473	36.015	1.00 27.79
ATOM	1912	CE3		C1075	27.923	20.731	38.161	1.00 29.11
ATOM	1913	CZ2		C1075	28.393	22.095	35.707	1.00 27.12
ATOM	1914	CZ3		C1075	29.172	21.338	37.861	1.00 27.92
ATOM	1915	CH2		C1075	29.394	22.010	36.640	1.00 26.04
ATOM	1916	N		C1076	21.729	19.503	40.206	1.00 38.82
ATOM	1917	CA		C1076	21.190	18.763	41.348	1.00 40.61
ATOM	1918	C		C1076	20.509	17.546	40.743	1.00 40.05
ATOM	1919	0		C1076	19.967	17.688	39.634	1.00 40.43
ATOM	1920	CB		C1076	20.272	19.608	42.208	1.00 42.35
ATOM	1921	CG		C1076	20.932	20.378	43.334	1.00 45.64
ATOM	1922	CD		C1076	20.106	21.505	43.893	1.00 49.70
ATOM	1923	NE		C1076	20.769	22.441	44.800	1.00 49.70
ATOM	1924	CZ		C1076	20.478			
ATOM	1925	NH1		C1076	19.508	23.723	45.050	1.00 51.66
ATOM	1926	NH2		C1076				1.00 50.03
ATOM	1927	Nn2		C1076	21.238	24.353	45.949	1.00 52.86
ATOM	1927	CA		C1077	20.598	16.392 15.200	41.374	1.00 41.20
ATOM	1929	C					40.818	1.00 42.65
ATOM	1930	0		C1077	18.447	15.393	40.555	1.00 38.60
ATOM	1931	CB		C1077	17.929	15.043	39.481	1.00 35.94
ATOM	1931	CG		C1077	20.198	13.968	41.695	1.00 45.87
111011	2002	-6	الاندف	C1077	20.013	12.643	40.962	1.00 50.08

ATOM	1933	CD	GLU	C1077	20.183	11.401	41.819	1.00 54.47
ATOM	1934	OEl	GLU	C1077	20.561	10.312	41.308	1.00 57.69
MOTA	1935	OE2	GLU	C1077	19.955	11.404	43.055	1.00 56.30
ATOM	1936	N	LYS	C1078	17.706	15.887	41.503	1.00 39.48
ATOM	1937	CA	LYS	C1078	16.243	16.090	41.262	1.00 40.94
ATOM	1938	С	LYS	C1078	16.079	17.369	40.455	1.00 40.21
MOTA	1939	0	LYS	C1078	16.480	18.449	40.854	1.00 38.01
MCTA	1940	CB	LYS	C1078	15.475	16.240	42.568	1.00 43.70
ATOM	1941	CG	LYS	C1078	15.829	15.188	43.605	1.00 46.67
ATOM	1942	CD	LYS	C1078	15.384	15.538	45.015	1.00 49.04
ATOM	1943	CE		C1078	15.414	14.237	45.826	1.00 53.53
ATOM	1944	NZ		C1078	14.894	14.422	47.213	1.00 55.30
ATOM	1945	N		C1079	15.476	17.282	39.288	1.00 38.88
ATOM	1946	CA		C1079	15.298	18.465	38.451	1.00 39.64
ATOM	1947	C		C1079	14.654	19.621	39.182	1.00 40.23
ATOM	1948	0		C1079	15.091	20.778	39.078	1.00 39.41
ATOM	1949	CB		C1079	14.521	17.924	37.259	1.00 36.96
ATOM	1950	CG		C1079	14.929	16.461	37.199	1.00 35.65
ATOM	1951	CD		C1079	14.988	16.035	38.647	1.00 36.92
ATOM	1952	N		C1080	13.657	19.387	40.028	1.00 41.92
ATOM	1953	CA		C1080	12.882	20.406		1.00 41.92
							40.717	
ATOM	1954	C		C1080	13.587	21.140	41.824	1.00 43.51
ATOM	1955	0		C1080	13.109	22.140	42.388	1.00 43.12
ATOM	1956	CB		C1080	11.505	19.831	41.176	1.00 45.60
ATOM	1957	CG		C1080	11.697	18.722	42.194	1.00 47.84
ATOM	1958	CD1		C1080	11.973	18.993	43.531	1.00 49.35
ATOM	1959	CD2		C1080	11.636	17.389	41.798	1.00 49.13
MOTA	1960	CEl		C1080	12.146	17.958	44.445	1.00 50.14
ATOM	1961	CE2		C1080	11.806	16.370	42.704	1.00 50.24
MOTA	1962	CZ		C1080	12.058	16.656	44.030	1.00 50.60
ATOM	1963	OH		C1080	12.242	15.597	44.908	1.00 53.21
MOTA	1964	N		C1081	14.799	20.700	42.144	1.00 44.60
MOTA	1965	CA		C1081	15.638	21.420	43.102	1.00 44.07
MOTA	1966	C		C1081	16.559	22.432	42.419	1.00 40.19
ATOM	1967	0		C1081	17.250	23.137	43.126	1.00 37.60
ATOM	1968	CB		C1081	16.508	20 467	43.922	1.00 45.52
MOTA	1969	CG		C1081	15.648	19.808	45.014	1.00 50.79
ATOM	1970	CD	GLU	C1081	16.627	18.944	45.789	1.00 54.16
MOTA	1971	OE1	GLU	C1081	16.879	19.248	46.968	1.00 58.46
MOTA	1972	OE2	GLU	C1081	17.210	17.991	45.250	1.00 55.69
ATOM	1973	N	ARG	C1082	16.647	22.458	41.105	1.00 39.28
ATOM	1974	CA	ARG	C1082	17.497	23.363	40.367	1.00 37.58
MOTA	1975	C	ARG	C1082	16.828	24.740	40.394	1.00 38.63
MOTA	1976	0	ARG	C1082	15.612	24.910	40.383	1.00 40.38
ATOM	1977	CB	ARG	C1082	17.704	22.926	38.895	1.00 36.08
ATOM	1978	CG	ARG	C1082	18.469	21.599	38.779	1.00 36.20
ATOM	1979	CD	ARG	C1082	18.609	20.955	37.417	1.00 33.59
ATOM	1980	NE	ARG	C1082	18.832	19.501	37.535	1.00 34.00
ATOM	1981	CZ		C1082	18.469	18.515	36.714	1.00 32.08
ATOM	1982	NH1		C1082	17.822	18.762	35.569	1.00 31.72
MOTA	1983	NH2		C1082	18.708	17.204	36.908	1.00 31.86
ATOM	1984	N		C1083	17.667	25.772	40.289	1.00 34.94
ATOM	1985	CA		C1083	17.201	27.135	40.253	1.00 32.78
ATOM	1986	C		C1083	16.556	27.432	38.912	1.00 32.70
ATOM	1987	ō		C1083	16.641	26.652	37.947	1.00 31.92
ATOM	1988	CB		C1083	18.446	28.006	40.398	1.00 27.76
ATOM	1989	CG		C1083	19.621	27.077	40.186	1.00 30.28
			. 1.0	01003	10.021	27.071		1.00 30.20

19.139 25.661 40.404 1.00 32.35 15.816 28.558 38.933 1.00 31.68 15.199 29.032 37.705 1.00 31.93 16.201 30.014 37.080 1.00 31.87 16.210 30.014 37.080 1.00 31.87 13.873 29.704 38.085 1.00 31.83 14.132 31.022 38.595 1.00 32.90 16.099 30.275 35.783 1.00 30.49 16.882 31.203 35.046 1.00 31.87 16.731 32.620 35.646 1.00 35.04 17.778 33.269 35.568 1.00 34.20 16.631 31.270 33.553 1.00 34.79 16.631 31.270 33.553 1.00 29.79 MOTA 1990 CD PRO C1083 ATOM 1991 N SER C1084 1992 CA ATOM SER C1084 1993 C ATOM SER C1084 1994 0 SER C1084 ATOM 1995 CB SER C1084 ATOM ATOM 1996 OG SER C1084 MOTA 1997 N PHE C1085 ATOM 1998 CA PHE C1085 ATOM 1999 C PHE C1085 2000 O PHE C1085 ATOM 2001 CB PHE C1085 16.631 31.270 33.533 1.00 29.72 ATOM ATOM 2002 CG PHE C1085 17.113 30.035 32.829 1.00 29.58 ATOM 2003 CD1 PHE C1085 16.278 29.113 32.259 1.00 27.05 ATOM 2004 CD2 PHE C1085 18.513 29.847 32.765 1.00 28.92 ATOM 2005 CE1 PHE C1085 16.764 28.002 31.606 1.00 29.03 18.999 28.739 32.078 1.00 31.04 MOTA 2006 CE2 PHE C1085 MOTA 2007 CZ PHE C1085 18.172 27.810 31.537 1.00 29.42 200B N ALA C1086 15.538 32.967 36.152 1.00 34.52 ATOM 15.461 34.251 36.811 1.00 34.52 15.461 34.251 36.811 1.00 36.63 16.330 34.297 38.053 1.00 35.05 16.940 35.370 38.305 1.00 33.03 13.991 34.579 37.178 1.00 36.02 2009 CA ALA C1086 ATOM 2010 C ATOM ALA C1086 ATOM 2011 0 ALA C1086 13.991 34.579 37.178 1.00 36.02 16.403 33.210 38.808 1.00 37.34 48 17.187 33.187 40.043 1.00 37.34 18.692 33.172 39.718 1.00 36.23 19.488 33.831 40.397 1.00 34.12 16.898 31.991 40.963 1.00 39.18 15.465 21.766 41.372 1.00 41.05 15.181 30.507 42.185 1.00 41.95 14.644 30.647 43.307 1.00 43.26 15.463 29.299 41.755 1.00 38.28 19.023 32.489 38.609 1.00 36.91 20.421 32.470 38.143 1.00 34.96 20.850 33.891 37.730 1.00 36.64 21.994 43.10 37.999 1.00 38.66 20.707 31.497 37.017 1.00 31.65 20.729 30.014 37.479 1.00 22.45 20.354 29.149 36.296 1.00 36.93 20.288 36.010 36.296 1.00 38.98 20.286 37.37 1.00 36.93 20.288 36.010 36.44 1.00 34.95 20.288 36.010 36.471 1.00 32.45 20.288 36.010 36.471 1.00 32.45 20.288 36.010 36.471 1.00 38.78 20.288 36.010 36.471 1.00 38.78 20.288 36.010 36.471 1.00 38.78 20.288 36.010 36.471 1.00 38.78 20.288 36.010 36.471 1.00 38.78 20.288 36.010 36.471 1.00 38.78 20.288 36.010 36.471 1.00 38.78 20.584 37.812 1.03 39.65 21.396 37.812 37.832 1.00 39.65 21.396 37.812 37.832 1.00 39.65 21.396 37.892 35.087 1.00 38.19 19.192 36.562 35.727 1.00 39.78 19.421 37.938 35.087 1.00 41.64 20.497 37.892 34.014 1.00 39.98 18.113 38.470 34.892 1.00 40.00 19.730 36.740 38.902 1.00 41.428 21.247 37.342 40.727 1.00 43.72 20.488 38.898 41 115 1.00 43.77 20.488 38.8 MOTA 2012 CB ALA C1086 2013 N GLN C1087 ATOM ATOM 2014 CA GLN C1087 ATOM 2015 C GLN C1087 ATOM 2016 0 GLN C1087 MOTA 2017 CB GLN C1087 ATOM 2018 CG GLN C1087 ATOM 2019 CD GLN C1087 ATOM 2020 OE1 GLN C1087 ATOM 2021 NE2 GLN C1087 ATOM 2022 N ILE C1088 ATOM 2023 CA ILE C1088 ATOM 2024 C ILE C1088 ATOM 2025 0 ILE C1088 ATOM 2026 CB ILE C1088 MOTA 2027 CG1 ILE C1088 ATCM 2028 CG2 ILE C1088 2029 CD1 ILE C1088 ATOM 2030 N LEU C1089 MOTA 2031 CA LEU C1089 2032 C LEU C1089 ATOM MOTA MOTA 2033 0 LEU C1089 2034 CB LEU C1089 MOTA 2035 CG LEU C1089 MOTA ATOM 2036 CD1 LEU C1089 ATOM 2037 CD2 LEU C1089 VAL C1090 ATOM 2038 N ATOM 2039 CA VAL C1090 VAL C1090 MOTA 2040 C 21.247 37.342 40.727 1.00 43.77 ATOM 2041 0 VAL C1090 21.948 38.289 41.115 1.00 45.25 MOTA 2042 CB VAL C1090 19.139 38.123 42.387 1.00 44.41 19.139 38.123 42.387 1.00 45.32 17.422 37.989 40.595 1.00 45.38 21.634 36.074 40.924 1.00 43.36 22.901 18.917 17.51 18,759 37,424 41,081 1.00 44,41 ATOM 2043 CG1 VAL C1090 ATOM 2044 CG2 VAL C1090 2045 N SER C1091 ATOM ATOM 2046 CA SER C1091 22.921 35.817 41.543 1.00 45.59

ATON	2047	С	SEF	C1091	24	.044	36.357	40.663	1 00	43.29
ATOM	2048	0	SEF	C1091		. 987	36.921	41.231		43.04
ATOM	2049	CB	SEF	C1091		.056	34.332	41.946		48.54
ATOM	2050	OG	SEF	C1091	22	.563	33.588	40.846		54.84
ATOM	2051	N	LEU	C1092	23	.971	36.337	39.335		38.97
MOTA	2052	CA	LEU	C1092	25	.098	36.849	38.570		37.84
ATOM	2053	C	LEU	C1092	25	.118	38.383	38.604		39.82
ATOM	2054	0	LEU	C1092	26	.207	38.957	38.627		35.95
ATOM	2055	CB	LEU	C1092	25	.098	36.309	37.150		35.04
ATOM	2056	CG	LEU	C1092	25	.301	34.789	36.982	1.00	33.88
ATOM	2057	CD1		C1092	24	.655	34.383	35.662	1.00	33.07
ATOM	2058	CD2		C1092		.773	34.446	37.016	1.00	34.04
MOTA	2059	N		C1093		.942	39.039	38.597	1.00	41.48
ATOM	2060	CA		C1093		.920	40.525	38.641	1.00	43.61
ATOM	2061	C		C1093		.527	41.074	39.936	1.00	44.92
ATOM MOTA	2062	0		C1093		.166	42.135	39.946		44.64
	2063	CB		C1093		.509	41.084	38.434		42.95
ATOM	2064	CG		C1093		.996	41.095	37.021		44.32
MOTA	2065	OD1		C1093		.771	41.140	36.726		46.00
ATOM	2066 2067	ND2		C1093		. 859	41.098	36.023		43.94
ATOM	2068	N CA	ARG			.374	40.336	41.043		46.27
ATOM	2069	CA		C1094 C1094		.957	40.724	42.334		47.34
ATOM	2070	0		C1094		.473	40.529	42.302		47.18
ATOM	2071	CB		C1094		.308	41.386	42.683		48.73
ATOM	2072	CG		C1094		.207	39.952	43.397		48.52
ATOM	2073	CD		C1094		.600 .893	40.135 39.506	44.831		53.04
ATOM	2074	NE		C1094		.811	38.266	45.266 46.057	1.00	55.51 58.34
ATOM	2075	CZ		C1094		.945	37.595	46.057		58.34
ATOM	2076	NH1		C1094		.144	37.993	45.942	1.00	58.67
ATOM	2077	NH2		C1094		. 892	36.486	47.071	1.00	
ATOM	2078	N	MET	C1095	26	.945	39.465	41.654	1.00	43.61
ATOM	2079	CA	MET	C1095		.378	39.288	41.439		41.53
ATOM	2080	С	MET	C1095	28	.854	40.419	40.535	1.00	37.96
ATOM	2081	0	MET	C1095	29	. 993	40.855	40.670	1.00	39.00
ATOM	2082	CB	MET	C1095	28.	.772	37.969	40.755	1.00	39.83
ATOM	2083	CG	MET	C1095	28	.636	36.767	41.644	1.00	42.24
ATOM	2084	SD		C1095	28.	.588	35.160	40.819	1.00	43.52
ATOM	2085	CE	MET	C1095		. 492	34.284	42.084	1.00	43.64
ATOM ATOM	2086	N		C1096		.128	40.770	39.489	1.00	38.63
ATOM	2087	CA		C1096		.592	41.811	38.583		40.32
ATOM	2088	0		C1096		726	43.159	39.300		45.56
ATOM	2099	CB		C1096		676	43.913	39.027		43.98
ATOM	2091	CG		C1096 C1096		705	41.881	37.363	1.00	38.78
ATOM	2092			C1096		859	40.853	36.254		36.87
ATOM	2093			C1096		623	40.917	35.364		37.20
ATOM	2094	N		C1096		.157	41.041	35.484		36.07
ATOM	2095	CA		C1097		911	43.531	40.207		50.71
ATOM	2096	C		C1097		997	44.809	40.888	1.00	56.21
ATOM	2097	0		C1097		115	46.249	42.308		57.95
ATOM	2098	CB		C1097		511	45.083	41.496		58.28 59.17
ATOM	2099	CG		C1097		588	45.556	40.362	1.00	62.97
ATOM	2100	CD		C1097		880	46.999	39.984		65.89
MOTA	2101	OE1		C1097		772	47.604	40.633	1.00	67.34
ATOM	2102			C1097		159	47.465	39.064	1.00	68.13
ATOM	2103	N		C1098		832	44.134	42.340		59.64
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ATOM 2105 C GLU C1098 32.317 44.135 42.709 1.0 ATOM 2106 O GLU C1098 30.721 43.618 44.546 1.0 ATOM 2107 CB GLU C1098 30.721 43.618 44.546 1.0 ATOM 2108 CG GLU C1098 30.447 42.441 44.299 1.0 ATOM 2110 OEI GLU C1098 30.447 42.441 44.299 1.0 ATOM 2110 OEI GLU C1098 30.447 42.441 44.299 1.0 ATOM 2110 OEI GLU C1098 30.447 42.441 44.299 1.0 ATOM 2111 OEI GLU C1098 30.447 42.441 44.299 1.0 ATOM 2112 N ARG C1099 33.234 45.047 45.616 1.0 ATOM 2113 CA ARG C1099 34.637 45.044 42.675 1.0 ATOM 2113 CA ARG C1099 34.637 45.044 42.675 1.0 ATOM 2114 C ARG C1099 35.404 43.736 42.782 1.0 ATOM 2115 O ARG C1099 35.404 43.736 42.782 1.0 ATOM 2116 CB ARG C1099 35.404 43.655 42.072 1.0 ATOM 2117 N LYS C1100 35.024 42.747 43.594 1.0 ATOM 2118 CA LYS C1100 35.024 42.747 43.594 1.0 ATOM 2119 C LYS C1100 35.034 41.056 43.624 1.0 ATOM 2120 C LYS C1100 35.881 40.863 42.288 1.0 ATOM 2121 CB LYS C1100 35.881 40.863 42.288 1.0 ATOM 2121 CB LYS C1100 35.831 41.060 41.366 1.0 ATOM 2122 CG LYS C1100 35.931 41.060 41.366 1.0 ATOM 2123 CD LYS C1100 34.550 39.418 44.451 1.0 ATOM 2124 CE LYS C1100 34.923 37.780 46.342 1.0 ATOM 2125 NZ LYS C1100 34.255 36.502 46.768 1.0 ATOM 2126 N THR C1101 36.911 40.037 42.055 1.0 ATOM 2127 CA THR C1101 36.911 40.037 42.055 1.0 ATOM 2128 C THR C1101 36.911 40.037 42.055 1.0 ATOM 2129 O THR C1101 36.911 40.037 42.055 1.0 ATOM 2130 CB THR C1101 38.694 39.327 40.489 1.0 ATOM 2131 CA THR C1101 38.694 39.327 40.489 1.0 ATOM 2133 N TYR C1102 35.864 37.355 40.667 1.0 ATOM 2133 CB THR C1101 38.694 39.327 40.489 1.0 ATOM 2133 CB THR C1101 38.694 39.327 40.489 1.0 ATOM 2134 CA THR C1101 38.694 39.327 40.489 1.0 ATOM 2135 C TYR C1102 33.858 35.910 40.007 1.0 ATOM 2136 C TYR C1102 33.694 39.327 40.489 1.0 ATOM 2137 CB THR C1101 38.694 39.327 40.489 1.0 ATOM 2138 CG TYR C1102 33.694 39.327 40.489 1.0 ATOM 2139 CB THR C1101 38.694 39.327 40.489 1.0 ATOM 2135 C TYR C1102 33.695 35.932 42.296 1.0 ATOM 2136 C TYR C1102 33.695 35.932 42.296 1.0 ATOM 2137 CB TYR C1102 33.695 35.932 42.296 1.0 ATOM 2140 CB TYR C1102 33.696 35.993 43.48	
ATOM 2105 C GLU C1098 32.317 44.135 42.709 1.0 ATOM 2106 O GLU C1098 30.721 43.618 44.546 1.0 ATOM 2107 CB GLU C1098 30.721 43.618 44.546 1.0 ATOM 2108 CG GLU C1098 30.447 42.441 44.299 1.0 ATOM 2110 OEI GLU C1098 30.447 42.441 44.299 1.0 ATOM 2110 OEI GLU C1098 30.447 42.441 44.299 1.0 ATOM 2110 OEI GLU C1098 30.447 42.441 44.299 1.0 ATOM 2111 OEI GLU C1098 30.447 42.441 44.299 1.0 ATOM 2112 N ARG C1099 33.234 45.047 45.616 1.0 ATOM 2113 CA ARG C1099 34.637 45.044 42.675 1.0 ATOM 2113 CA ARG C1099 34.637 45.044 42.675 1.0 ATOM 2114 C ARG C1099 35.404 43.736 42.782 1.0 ATOM 2115 O ARG C1099 35.404 43.736 42.782 1.0 ATOM 2116 CB ARG C1099 35.404 43.655 42.072 1.0 ATOM 2117 N LYS C1100 35.024 42.747 43.594 1.0 ATOM 2118 CA LYS C1100 35.024 42.747 43.594 1.0 ATOM 2119 C LYS C1100 35.034 41.056 43.624 1.0 ATOM 2120 C LYS C1100 35.881 40.863 42.288 1.0 ATOM 2121 CB LYS C1100 35.881 40.863 42.288 1.0 ATOM 2121 CB LYS C1100 35.831 41.060 41.366 1.0 ATOM 2122 CG LYS C1100 35.931 41.060 41.366 1.0 ATOM 2123 CD LYS C1100 34.550 39.418 44.451 1.0 ATOM 2124 CE LYS C1100 34.923 37.780 46.342 1.0 ATOM 2125 NZ LYS C1100 34.255 36.502 46.768 1.0 ATOM 2126 N THR C1101 36.911 40.037 42.055 1.0 ATOM 2127 CA THR C1101 36.911 40.037 42.055 1.0 ATOM 2128 C THR C1101 36.911 40.037 42.055 1.0 ATOM 2129 O THR C1101 36.911 40.037 42.055 1.0 ATOM 2130 CB THR C1101 38.694 39.327 40.489 1.0 ATOM 2131 CA THR C1101 38.694 39.327 40.489 1.0 ATOM 2133 N TYR C1102 35.864 37.355 40.667 1.0 ATOM 2133 CB THR C1101 38.694 39.327 40.489 1.0 ATOM 2133 CB THR C1101 38.694 39.327 40.489 1.0 ATOM 2134 CA THR C1101 38.694 39.327 40.489 1.0 ATOM 2135 C TYR C1102 33.858 35.910 40.007 1.0 ATOM 2136 C TYR C1102 33.694 39.327 40.489 1.0 ATOM 2137 CB THR C1101 38.694 39.327 40.489 1.0 ATOM 2138 CG TYR C1102 33.694 39.327 40.489 1.0 ATOM 2139 CB THR C1101 38.694 39.327 40.489 1.0 ATOM 2135 C TYR C1102 33.695 35.932 42.296 1.0 ATOM 2136 C TYR C1102 33.695 35.932 42.296 1.0 ATOM 2137 CB TYR C1102 33.695 35.932 42.296 1.0 ATOM 2140 CB TYR C1102 33.696 35.993 43.48	00 62.30
ATOM 2107 CB GUU C1098 32.699 43.098 42.165 1.0 ATOM 2107 CB GUU C1098 30.721 43.618 44.546 1.0 ATOM 2108 CG GUU C1098 30.447 42.141 44.289 1.0 ATOM 2110 OEI GUU C1098 30.147 42.141 44.289 1.0 ATOM 2111 OEE GUU C1098 30.147 42.141 44.289 1.0 ATOM 2111 OEE GUU C1098 30.943 40.587 46.262 1.0 ATOM 2112 N ARG C1099 33.943 40.587 46.262 1.0 ATOM 2113 CA ARG C1099 33.94 45.047 43.011 1.0 ATOM 2114 C ARG C1099 35.4637 45.047 43.011 1.0 ATOM 2115 O ARG C1099 35.4637 45.044 42.675 1.0 ATOM 2116 CB ARG C1099 35.404 43.763 42.782 1.0 ATOM 2117 N LYS C1100 35.024 42.747 43.594 1.0 ATOM 2118 CA LYS C1100 35.024 42.747 43.594 1.0 ATOM 2119 C LYS C1100 35.843 41.536 42.782 1.0 ATOM 2120 O LYS C1100 35.843 41.536 42.782 1.0 ATOM 2121 CB LYS C1100 35.843 41.536 42.782 1.0 ATOM 2121 CB LYS C1100 35.843 41.536 42.782 1.0 ATOM 2122 CG LYS C1100 35.083 41.536 42.782 1.0 ATOM 2121 CB LYS C1100 35.083 41.536 42.782 1.0 ATOM 2122 CG LYS C1100 35.083 41.536 42.782 1.0 ATOM 2123 CD LYS C1100 34.580 39.418 44.451 1.0 ATOM 2124 CE LYS C1100 34.580 39.418 44.451 1.0 ATOM 2126 N THR C1101 36.914 40.629 44.760 1.0 ATOM 2127 CA THR C1101 36.914 40.037 42.055 1.0 ATOM 2128 C THR C1101 36.914 40.037 42.055 1.0 ATOM 2128 C THR C1101 36.914 40.037 42.055 1.0 ATOM 2128 C THR C1101 36.914 40.037 42.055 1.0 ATOM 2128 C THR C1101 36.914 40.037 42.055 1.0 ATOM 2128 C THR C1101 36.946 37.355 40.640 1.0 ATOM 2129 O THR C1101 36.946 37.355 40.640 1.0 ATOM 2131 CGI THR C1101 38.694 37.352 40.696 1.0 ATOM 2131 CGI THR C1101 38.694 37.352 40.696 1.0 ATOM 2131 CGI THR C1101 38.694 37.352 40.696 1.0 ATOM 2132 CGI CYR C1100 31.909 40.606 39.999 1.0 ATOM 2131 CGI THR C1101 38.694 37.352 40.696 1.0 ATOM 2131 CGI THR C1101 38.694 37.352 40.696 1.0 ATOM 2133 CGI THR C1101 38.694 37.352 40.696 1.0 ATOM 2134 CCI THR C1101 38.694 39.327 40.489 1.0 ATOM 2135 CGI THR C1101 38.694 37.354 40.017 1.0 ATOM 2136 C TYR C1102 33.686 39.994 1.0 ATOM 2137 CA THR C1101 38.694 39.327 40.489 1.0 ATOM 2138 CGI TYR C1102 33.696 38.590 40.006 39.999 1.0 ATOM 2139 CDI THR C1101 38.694	00 61.47
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ATOM 2138 CG TYR C1102 33.074 36.622 41.174 1.0 ATOM 2139 CDI TYR C1102 32.609 35.932 42.296 1.0 ATOM 2140 CD2 TYR C1102 32.609 35.932 42.296 1.0 ATOM 2141 CBI TYR C1102 32.609 35.932 42.296 1.0 ATOM 2141 CBI TYR C1102 32.609 35.932 42.296 1.0 ATOM 2142 CB2 TYR C1102 31.904 36.580 43.294 1.0 ATOM 2143 CZ TYR C1102 31.904 36.580 43.294 1.0 ATOM 2144 OH TYR C1102 30.961 38.602 44.148 1.0 ATOM 2145 N VAL C1103 36.753 35.276 38.570 1.0 ATOM 2146 CA VAL C1103 36.753 35.276 38.570 1.0 ATOM 2147 C VAL C1103 36.953 35.061 37.561 1.0 ATOM 2148 O VAL C1103 37.580 34.400 37.772 1.0 ATOM 2149 CB VAL C1103 37.980 36.043 36.864 1.0 ATOM 2149 CB VAL C1103 37.980 36.043 36.864 1.0 ATOM 2150 CG1 VAL C1103 37.938 35.061 37.561 1.0 ATOM 2151 CG2 VAL C1103 37.938 34.042 36.390 1.0 ATOM 2151 CG2 VAL C1103 37.938 33.463 36.464 1.0 ATOM 2151 CG2 VAL C1103 37.938 34.042 36.390 1.0 ATOM 2151 CG2 VAL C1103 37.938 34.042 36.390 1.0 ATOM 2151 CG2 VAL C1103 37.938 38.603 35.738 1.0 ATOM 2152 N ASN C1104 39.993 34.484 38.154 1.0 ATOM 2153 CA ASN C1104 41.366 34.972 38.131 1.0 ATOM 2155 C ASN C1104 42.066 34.752 36.765 1.0 ATOM 2155 C BASN C1104 42.016 33.569 36.390 1.0 ATOM 2155 C BASN C1104 42.161 33.569 36.390 1.0 ATOM 2155 C BASN C1104 42.161 33.569 36.390 1.0 ATOM 2155 C BASN C1104 42.161 33.569 36.390 1.0 ATOM 2155 C BASN C1104 42.161 33.569 39.140 1.0 ATOM 2156 CB ASN C1104 42.161 33.569 39.140 1.0 ATOM 2157 CG ASN C1104 42.161 33.569 39.140 1.0 ATOM 2158 CD1 ASN C1104 42.161 33.569 39.140 1.0 ATOM 2157 CG ASN C1104 43.661 34.686 39.140 1.0	0 38.06
ATOM 2139 CD1 TYR C1102 32.812 37.986 41.085 1.08 ATOM 2140 CD2 TYR C1102 32.609 35.932 42.296 1.00 ATOM 2141 CB1 TYR C1102 32.107 38.642 42.966 1.00 ATOM 2142 CB2 TYR C1102 31.904 36.580 43.294 1.00 ATOM 2143 CZ TYR C1102 31.904 36.580 43.128 1.00 ATOM 2145 CB2 TYR C1102 31.904 36.580 43.128 1.00 ATOM 2145 N VAL C1103 36.753 35.276 38.570 1.00 ATOM 2145 N VAL C1103 37.580 34.400 37.772 1.00 ATOM 2146 CA VAL C1103 37.580 34.400 37.772 1.00 ATOM 2147 C VAL C1103 38.963 35.061 37.561 1.00 ATOM 2148 O VAL C1103 38.963 35.061 37.561 1.00 ATOM 2149 CB VAL C1103 37.038 34.042 36.390 1.00 ATOM 2150 CG1 VAL C1103 37.938 34.042 36.390 1.00 ATOM 2150 CG1 VAL C1103 37.938 34.042 36.390 1.00 ATOM 2151 CG2 VAL C1103 37.938 34.042 36.390 1.00 ATOM 2152 N ANN C1104 37.993 34.484 38.154 1.00 ATOM 2153 CA ASN C1104 41.366 34.972 38.131 1.00 ATOM 2155 C ASN C1104 42.006 34.745 36.765 1.00 ATOM 2155 CA ASN C1104 42.006 34.745 36.765 1.00 ATOM 2155 CB ASN C1104 42.101 33.569 36.390 1.00 ATOM 2155 CB ASN C1104 42.101 33.569 36.390 1.00 ATOM 2155 CB ASN C1104 42.212 34.184 39.143 1.00 ATOM 2155 CB ASN C1104 42.212 34.184 39.143 1.00 ATOM 2155 CB ASN C1104 42.212 34.184 39.143 1.00 ATOM 2155 CB ASN C1104 42.212 34.184 39.143 1.00 ATOM 2155 CB ASN C1104 42.212 34.184 39.143 1.00 ATOM 2155 CB ASN C1104 42.616 34.566 34.972 36.396 34.00 34.	0 39.42
ATOM 2140 CD2 TYR C1102 32.009 35.932 42.296 1.0 ATOM 2141 CEI TYR C1102 32.107 38.642 42.061 1.0 ATOM 2142 CE2 TYR C1102 31.904 36.580 43.294 1.0 ATOM 2143 CZ TYR C1102 31.904 36.580 43.294 1.0 ATOM 2144 OR TYR C1102 31.672 37.936 43.168 1.0 ATOM 2145 N VAL C1103 30.961 38.602 44.148 1.0 ATOM 2146 CA VAL C1103 36.753 35.276 38.570 1.0 ATOM 2146 CA VAL C1103 36.753 35.276 38.570 1.0 ATOM 2147 C VAL C1103 36.963 35.061 37.561 1.0 ATOM 2148 O VAL C1103 39.970 36.083 36.684 1.0 ATOM 2149 CB VAL C1103 37.961 33.001 35.738 1.0 ATOM 2149 CB VAL C1103 37.961 33.001 35.738 1.0 ATOM 2150 CG1 VAL C1103 37.961 33.001 35.738 1.0 ATOM 2151 CG2 VAL C1103 37.961 33.463 36.439 1.0 ATOM 2152 N ASN C1104 39.993 34.484 38.154 1.0 ATOM 2153 CA ASN C1104 42.006 34.775 38.134 1.0 ATOM 2155 C ASN C1104 42.006 34.745 36.765 1.0 ATOM 2155 C ASN C1104 42.006 34.745 36.765 1.0 ATOM 2155 C ASN C1104 42.016 33.569 36.390 1.0 ATOM 2155 C ASN C1104 42.161 33.569 36.390 1.0 ATOM 2155 C ASN C1104 42.161 33.569 36.390 1.0 ATOM 2155 C ASN C1104 42.161 33.569 36.390 1.0 ATOM 2155 C ASN C1104 42.161 33.569 36.390 1.0 ATOM 2155 C ASN C1104 42.161 33.569 36.390 1.0 ATOM 2156 C ASN C1104 42.161 33.569 36.390 1.0 ATOM 2157 CG ASN C1104 42.163 33.591 38.841 1.0 ATOM 2158 CD ASN C1104 44.3661 34.686 39.140 1.0 ATOM 2158 CD ASN C1104 44.3661 34.686 39.140 1.0 ATOM 2158 CD ASN C1104 44.3661 34.888 39.143 1.0 ATOM 2158 CD ASN C1104 44.3661 34.888 39.143 1.0 ATOM 2158 CD ASN C1104 44.3661 34.888 39.143 1.0 ATOM 2158 CD ASN C1104 44.3661 34.888 39.143 1.0	0 40.49
ATOM 2141 CEL TYR C1102 32.107 38.642 42.061 1.0 ATOM 2142 CEZ TYR C1102 31.904 36.580 43.294 1.0 ATOM 2143 CZ TYR C1102 31.672 37.936 43.1268 1.0 ATOM 2144 OH TYR C1102 31.672 37.936 43.1268 1.0 ATOM 2145 N VAL C1103 30.961 38.602 44.148 1.0 ATOM 2145 N VAL C1103 36.753 35.276 38.570 1.0 ATOM 2146 CA VAL C1103 37.580 34.400 37.772 1.0 ATOM 2147 C VAL C1103 37.580 34.400 37.772 1.0 ATOM 2148 O VAL C1103 37.580 36.061 37.561 1.0 ATOM 2149 CB VAL C1103 37.038 34.042 36.390 1.0 ATOM 2150 CG1 VAL C1103 37.038 34.042 36.390 1.0 ATOM 2151 CG2 VAL C1103 37.938 34.042 36.390 1.0 ATOM 2152 N ASN C1104 37.938 34.484 38.154 1.0 ATOM 2153 CA ASN C1104 41.366 34.972 38.131 1.0 ATOM 2155 C ASN C1104 41.366 34.972 38.131 1.0 ATOM 2155 C ASN C1104 42.066 34.755 36.765 1.0 ATOM 2155 C B ASN C1104 42.061 33.569 36.390 1.0 ATOM 2155 C B ASN C1104 42.161 33.569 36.390 1.0 ATOM 2155 C B ASN C1104 42.161 33.569 36.390 1.0 ATOM 2155 C ASN C1104 42.161 33.569 36.390 1.0 ATOM 2155 C B ASN C1104 42.161 33.569 36.390 1.0 ATOM 2155 C B ASN C1104 42.161 33.569 36.390 1.0 ATOM 2155 C B ASN C1104 42.161 33.569 36.390 1.0 ATOM 2155 C B ASN C1104 42.161 33.569 36.390 1.0 ATOM 2155 C B ASN C1104 42.161 33.569 36.390 1.0 ATOM 2155 C B ASN C1104 42.161 33.569 36.390 1.0 ATOM 2157 CG ASN C1104 42.161 33.569 36.390 1.0 ATOM 2158 CD ASN C1104 43.661 33.591 38.841 1.0	0 40.49
ATOM 2142 CE2 TYR C1102 31.904 36.580 43.294 1.00 ATOM 2143 CZ TYR C1102 31.672 37.936 43.168 1.00 ATOM 2144 OH TYR C1102 30.961 38.602 44.148 1.00 ATOM 2145 N VAL C1103 36.753 35.276 38.570 1.00 ATOM 2146 CA VAL C1103 37.580 34.400 37.772 1.00 ATOM 2146 CA VAL C1103 37.580 34.400 37.772 1.00 ATOM 2147 C VAL C1103 38.963 35.061 37.561 1.00 ATOM 2148 O VAL C1103 39.070 36.083 36.864 1.00 ATOM 2149 CE VAL C1103 39.070 36.083 36.864 1.00 ATOM 2150 CG1 VAL C1103 37.038 34.042 36.390 1.00 ATOM 2151 CG2 VAL C1103 37.961 33.001 35.738 1.00 ATOM 2152 N ASN C1104 39.993 34.484 38.154 1.00 ATOM 2153 CA SN C1104 41.366 34.972 38.131 1.00 ATOM 2155 C ASN C1104 41.366 34.972 38.131 1.00 ATOM 2155 O ASN C1104 42.006 34.745 36.765 1.00 ATOM 2155 C ASN C1104 42.006 34.745 36.765 1.00 ATOM 2155 C ASN C1104 42.016 33.569 36.390 1.00 ATOM 2155 C ASN C1104 42.016 33.569 36.390 1.00 ATOM 2155 C ASN C1104 42.016 33.569 36.390 1.00 ATOM 2155 C ASN C1104 42.016 33.569 36.390 1.00 ATOM 2155 C ASN C1104 42.016 33.569 36.390 1.00 ATOM 2155 C ASN C1104 42.016 33.569 36.390 1.00 ATOM 2155 C ASN C1104 42.016 33.569 36.390 1.00 ATOM 2155 C ASN C1104 42.016 33.569 36.390 1.00 ATOM 2156 CB ASN C1104 42.016 33.569 39.140 1.00 ATOM 2157 CG ASN C1104 43.661 33.569 39.140 1.00	0 41.47
ATOM 2143 CZ TYR C1102 31.672 37.936 43.168 1.01 ATOM 2144 OH TYR C1102 30.961 38.602 44.148 1.01 ATOM 2145 N VAL C1103 36.753 35.276 38.570 1.01 ATOM 2146 CA VAL C1103 37.580 34.400 37.772 1.01 ATOM 2147 C VAL C1103 38.963 35.061 37.561 1.01 ATOM 2148 O VAL C1103 38.963 35.061 37.561 1.01 ATOM 2149 CB VAL C1103 37.038 34.042 36.390 1.01 ATOM 2150 CG1 VAL C1103 37.961 33.001 35.738 1.01 ATOM 2151 CG2 VAL C1103 37.961 33.001 35.738 1.01 ATOM 2151 CG2 VAL C1103 37.961 33.001 35.738 1.01 ATOM 2152 N ASN C1104 39.993 34.484 38.154 1.00 ATOM 2153 CA ASN C1104 41.366 34.972 38.131 1.01 ATOM 2155 C ASN C1104 42.016 34.755 36.765 1.01 ATOM 2155 C B ASN C1104 42.016 33.593 36.390 1.01 ATOM 2155 C B ASN C1104 42.016 34.755 36.795 1.01 ATOM 2155 C B ASN C1104 42.161 33.569 36.390 1.01 ATOM 2155 C B ASN C1104 42.161 33.569 36.390 1.01 ATOM 2157 CG ASN C1104 42.161 33.569 36.390 1.01 ATOM 2158 CB ASN C1104 42.161 33.569 39.140 1.01 ATOM 2157 CG ASN C1104 42.161 33.569 39.140 1.01 ATOM 2158 CD ASN C1104 42.161 33.569 39.140 1.01	0 41.47
ATOM 2144 OH TYR C1102 30.961 38.602 44.148 1.00 ATOM 2145 N VAL C1103 36.753 35.276 38.570 1.00 ATOM 2146 CA VAL C1103 37.580 34.400 37.772 1.00 ATOM 2147 C VAL C1103 38.963 35.061 37.561 1.00 ATOM 2148 O VAL C1103 38.963 35.061 37.561 1.00 ATOM 2148 O VAL C1103 38.963 35.061 37.561 1.00 ATOM 2149 CE VAL C1103 38.963 35.061 37.561 1.00 ATOM 2150 CG1 VAL C1103 37.038 34.042 36.390 1.00 ATOM 2151 CG2 VAL C1103 37.961 33.001 35.738 1.00 ATOM 2151 CG2 VAL C1103 35.597 33.463 36.439 1.00 ATOM 2152 N ASN C1104 39.993 34.484 38.154 1.00 ATOM 2153 CA ASN C1104 41.366 34.972 38.131 1.00 ATOM 2155 O ASN C1104 42.006 34.745 36.765 1.00 ATOM 2155 O ASN C1104 42.016 33.569 36.390 1.00 ATOM 2155 O ASN C1104 42.016 33.569 36.390 1.00 ATOM 2155 CB ASN C1104 42.161 33.569 36.390 1.00 ATOM 2155 CB ASN C1104 42.161 33.569 36.390 1.00 ATOM 2155 CB ASN C1104 42.161 33.569 36.390 1.00 ATOM 2155 CB ASN C1104 42.161 33.569 39.143 1.00 ATOM 2158 CD ASN C1104 42.663 33.918 38.841 1.00	0 42.72
ATOM 2145 N VAL C1103 36.753 35.276 38.570 1.00 ATOM 2146 CA VAL C1103 37.580 34.400 37.772 1.00 ATOM 2147 C VAL C1103 38.963 35.061 37.561 1.00 ATOM 2148 O VAL C1103 38.963 35.061 37.561 1.00 ATOM 2149 CB VAL C1103 39.070 36.083 36.364 1.00 ATOM 2150 CG1 VAL C1103 37.961 33.001 35.738 1.00 ATOM 2151 CG2 VAL C1103 37.961 33.001 35.738 1.00 ATOM 2152 N ASN C1104 39.993 34.484 38.154 1.00 ATOM 2153 CA ASN C1104 41.366 34.792 38.131 1.00 ATOM 2155 C ASN C1104 42.101 33.569 36.390 1.00 ATOM 2155 CB ASN C1104 42.101 33.569 36.390 1.00 ATOM 2155 CB ASN C1104 42.112 34.184 39.143 1.00 ATOM 2157 CG ASN C1104 42.212 34.184 39.143 1.00 ATOM 2158 CB ASN C1104 43.661 34.662 39.140 1.00 ATOM 2157 CG ASN C1104 43.661 34.662 39.140 1.00 ATOM 2158 CD1 ASN C1104 43.661 34.662 39.140 1.00 ATOM 2158 CD1 ASN C1104 43.661 34.662 39.140 1.00 ATOM 2158 CD1 ASN C1104 43.661 34.662 39.140 1.00 ATOM 2158 CD1 ASN C1104 43.661 34.662 39.140 1.00 ATOM 2158 CD1 ASN C1104 43.661 34.662 39.140 1.00 ATOM 2158 CD1 ASN C1104 43.661 34.662 39.140 1.00 ATOM 2158 CD1 ASN C1104 43.661 34.662 39.140 1.00 ATOM 2158 CD1 ASN C1104 43.661 34.662 39.140 1.00 ATOM 2158 CD1 ASN C1104 43.661 34.662 39.140 1.00 ATOM 2158 CD1 ASN C1104 43.661 34.662 39.140 1.00 ATOM 2158 CD1 ASN C1104 43.661 34.662 39.140 1.00 ATOM 2158 CD1 ASN C1104 43.661 34.662 39.140 1.00 ATOM 2158 CD1 ASN C1104 43.661 34.662 39.140 1.00 ATOM 2158 CD1 ASN C1104 43.661 34.662 39.140 1.00 ATOM 2158 CD1 ASN C1104 43.661 34.662 39.140 1.00 ATOM 2158 CD1 ASN C1104 43.661 34.662 39.140 1.00 ATOM 2158 CD1 ASN C1104	0 42.72
ATOM 2146 CA VAL C1103 37.580 34.400 37.772 1.00 ATOM 2147 C VAL C1103 38.963 35.061 37.561 1.00 ATOM 2148 O VAL C1103 38.963 35.061 37.561 1.00 ATOM 2149 CB VAL C1103 37.038 34.042 36.390 1.00 ATOM 2150 CG1 VAL C1103 37.038 34.042 36.390 1.00 ATOM 2150 CG2 VAL C1103 37.938 34.042 36.390 1.00 ATOM 2151 CG2 VAL C1103 37.937 33.463 36.439 1.00 ATOM 2152 N ASN C1104 35.597 33.463 36.439 1.00 ATOM 2153 CA ASN C1104 41.366 34.972 38.131 1.00 ATOM 2155 C ASN C1104 42.006 34.745 36.765 1.00 ATOM 2155 O ASN C1104 42.016 33.569 36.390 1.00 ATOM 2155 CB ASN C1104 42.112 34.184 39.143 1.00 ATOM 2157 CG ASN C1104 43.661 34.686 39.140 1.00 ATOM 2158 CD1 ASN C1104 43.661 34.686 39.140 1.00 ATOM 2158 CD1 ASN C1104 43.661 33.591 38.841 1.00 ATOM 2158 CD1 ASN C1104 44.630 33.9918 38.841 1.00 ATOM 2158 CD1 ASN C1104 44.630 33.9918 38.841 1.00 ATOM 2158 CD1 ASN C1104 44.630 33.9918 38.841 1.00 ATOM 2158 CD1 ASN C1104 44.630 33.9918 38.841 1.00 ATOM 2158 CD1 ASN C1104 44.630 33.9918 38.841 1.00 ATOM 2158 CD1 ASN C1104 44.630 33.9918 38.841 1.00 ATOM 2158 CD1 ASN C1104 44.630 33.9918 38.841 1.00 ATOM 2158 CD1 ASN C1104 44.630 33.9918 38.841 1.00 ATOM 2158 CD1 ASN C1104 44.630 33.9918 38.841 1.00 ATOM 2158 CD1 ASN C1104 44.630 33.9918 38.841 1.00 ATOM 2158 CD1 ASN C1104 44.630 33.9918 38.841 1.00 ATOM 2158 CD1 ASN C1104 44.630 33.9918 38.841 1.00 ATOM 2158 CD1 ASN C1104 44.630 33.9918 38.841 1.00 ATOM 2158 CD1 ASN C1104 44.630 33.9918 38.841 1.00 ATOM 2158 C	0 40.18
ATOM 2147 C VAL C1103 38.963 35.061 37.561 1.00 ATOM 2148 O VAL C1103 39.070 36.083 36.864 1.00 ATOM 2149 CB VAL C1103 37.038 34.042 36.390 1.00 ATOM 2150 CG1 VAL C1103 37.038 34.042 36.390 1.00 ATOM 2151 CG2 VAL C1103 37.961 33.001 35.738 1.00 ATOM 2151 CG2 VAL C1103 35.597 33.463 36.4399 1.00 ATOM 2152 N ASN C1104 39.993 34.484 38.154 1.00 ATOM 2153 CA ASN C1104 41.366 34.972 38.131 1.00 ATOM 2154 C ASN C1104 42.006 34.745 36.765 1.00 ATOM 2155 O ASN C1104 42.161 33.569 36.390 1.00 ATOM 2155 CB ASN C1104 42.161 33.569 36.390 1.00 ATOM 2156 CB ASN C1104 42.161 33.569 36.390 1.00 ATOM 2157 CG ASN C1104 42.161 33.569 39.143 1.00 ATOM 2158 CD ASN C1104 42.303 33.918 39.143 1.00 ATOM 2158 CD ASN C1104 44.613 36.30 38.841 1.00	0 38.79
ATOM 2148 O VAL C1103 39.070 36.083 36.864 1.00 ATOM 2149 CB VAL C1103 37.038 34.042 36.390 1.00 ATOM 2150 CG1 VAL C1103 37.961 33.001 35.738 1.00 ATOM 2151 CG2 VAL C1103 37.961 33.001 35.738 1.00 ATOM 2152 N ASN C1104 39.993 34.464 38.154 1.00 ATOM 2153 CA ASN C1104 41.366 34.972 38.131 1.00 ATOM 2154 C ASN C1104 42.066 34.745 36.765 1.00 ATOM 2155 O ASN C1104 42.061 33.569 36.390 1.00 ATOM 2155 C ASN C1104 42.161 33.569 36.390 1.00 ATOM 2155 C ASN C1104 42.161 33.569 36.390 1.00 ATOM 2156 CB ASN C1104 42.161 33.569 36.390 1.00 ATOM 2157 CG ASN C1104 42.161 33.666 39.140 1.00 ATOM 2158 OD1 ASN C1104 43.661 34.686 39.140 1.00	
ATOM 2149 CB VAL C1103 37.038 34.042 36.390 1.00 ATOM 2150 CG1 VAL C1103 37.961 33.001 35.738 1.00 ATOM 2151 CG2 VAL C1103 25.597 33.463 36.439 1.00 ATOM 2152 N ASN C1104 39.993 34.484 38.154 1.00 ATOM 2153 CA SN C1104 41.366 34.972 38.131 1.00 ATOM 2154 C ASN C1104 42.006 34.745 36.765 1.00 ATOM 2155 O ASN C1104 42.006 34.745 36.765 1.00 ATOM 2155 CB ASN C1104 42.016 33.569 36.390 1.00 ATOM 2156 CB ASN C1104 42.11 33.569 36.390 1.00 ATOM 2158 CD1 ASN C1104 42.11 33.560 39.143 1.00 ATOM 2158 CB ASN C1104 42.60 33.3918 38.841 1.00	0 40.96 0 41.22
ATOM 2150 CG1 VAL C1103 37.961 33.001 35.738 1.00 ATOM 2151 CG2 VAL C1103 35.597 33.463 36.439 1.00 ATOM 2152 N ASN C1104 39.993 34.484 38.154 1.00 ATOM 2153 CA ASN C1104 41.366 34.972 38.131 1.00 ATOM 2154 C ASN C1104 42.006 34.745 36.765 1.00 ATOM 2155 O ASN C1104 42.161 33.569 36.390 1.00 ATOM 2155 CB ASN C1104 42.161 33.569 36.390 1.00 ATOM 2155 CB ASN C1104 42.161 34.666 39.140 1.00 ATOM 2157 CG ASN C1104 43.661 34.666 39.140 1.00 ATOM 2158 CD1 ASN C1104 44.630 33.918 38.841 1.00	0 39.03
ATOM 2151 CG2 VAL C1103 35.597 33.463 36.439 1.00 ATOM 2152 N ASN C1104 39.993 34.484 38.154 1.00 ATOM 2153 CA ASN C1104 41.366 34.972 38.131 1.00 ATOM 2155 C ASN C1104 42.006 34.745 36.765 1.00 ATOM 2155 O ASN C1104 42.016 33.569 36.390 1.00 ATOM 2155 CB ASN C1104 42.11 33.569 36.390 1.00 ATOM 2156 CB ASN C1104 42.12 34.184 39.143 1.00 ATOM 2157 CG ASN C1104 43.661 34.686 39.140 1.00 ATOM 2158 CD1 ASN C1104 44.630 33.918 38.841 1.00	
ATOM 2152 N ASN C1104 39.993 34.484 38.154 1.00 ATOM 2153 CA ASN C1104 41.366 34.972 38.131 1.00 ATOM 2154 C ASN C1104 42.006 34.745 36.765 1.00 ATOM 2155 O ASN C1104 42.161 33.569 36.390 1.00 ATOM 2156 CB ASN C1104 42.161 33.569 36.390 1.00 ATOM 2157 CG ASN C1104 42.212 34.184 39.143 1.00 ATOM 2158 OD1 ASN C1104 43.661 34.686 39.140 1.00	
ATOM 2157 CA ASN C1104 41.366 34.972 38.131 1.00 ATOM 2154 C ASN C1104 42.066 34.745 36.765 1.00 ATOM 2155 O ASN C1104 42.161 33.569 36.390 1.00 ATOM 2156 CB ASN C1104 42.161 33.569 36.390 1.00 ATOM 2157 CG ASN C1104 42.121 34.184 39.143 1.00 ATOM 2158 OD1 ASN C1104 43.661 34.686 39.140 1.00	0 36.18
ATOM 2154 C ASN C1104 42.066 34.745 36.765 1.00 ATOM 2155 O ASN C1104 42.161 33.569 36.390 1.00 ATOM 2156 CB ASN C1104 42.161 33.569 36.390 1.00 ATOM 2157 CG ASN C1104 42.212 34.184 39.143 1.00 ATOM 2158 OD1 ASN C1104 43.661 34.686 39.140 1.00	
ATOM 2155 O ASN C1104 42.161 33.569 36.390 1.00 ATOM 2156 CB ASN C1104 42.212 34.184 39.143 1.00 ATOM 2157 CG ASN C1104 43.661 34.686 39.140 1.00 ATOM 2158 OD1 ASN C1104 44.630 33.918 38.841 1.00	0 43.68
ATOM 2156 CB ASN C1104 42.212 34.184 39.143 1.00 ATOM 2157 CG ASN C1104 43.661 34.686 39.140 1.00 ATOM 2158 CD1 ASN C1104 44.630 33.918 38.841 1.00	0 42.39
ATOM 2157 CG ASN C1104 43.661 34.686 39.140 1.00 ATOM 2158 OD1 ASN C1104 44.630 33.918 38.841 1.00	0 46.58
ATOM 2158 OD1 ASN C1104 44.630 33.918 38.841 1.00	0 44.69
AMON 0350 30.041 1.00	
	0 49.14
7mov 23.00 N	0 47.59
	0 38.71

OWNER

ATOM	2161	CA	THR	C1105	42.937	35.664	34.723	1.00 38.30
ATOM	2162	С		C1105	44.389	36.105	34.806	1.00 37.67
MOTA	2163	ō		C1105	44.998	36.087	33.725	1.00 39.99
ATOM	2164	CB		C1105	42.272	36.465	33.585	1.00 36.40
ATOM	2165	OG1		C1105	42.212	37.883	33.885	1.00 38.39
ATOM	2166	CG2		C1105	40.875	35.906	33.439	1.00 35.66
ATOM	2167	N		C1106	44.918	36.386	35.989	1.00 39.77
ATOM	2168	CA		C1106	46.306	36.915	36.002	1.00 43.19
ATOM	2169	C	THE		47.368	35.852	36.199	1.00 44.10
ATOM	2170	0		C1106	47.129	34.854	36.896	1.00 45.27
ATOM	2171	CB		C1106	46.445	38.022	37.058	1.00 47.23
ATOM	2172	0G1		C1106	46.210	37.460	38.369	1.00 52.99
ATOM	2173	CG2		C1106	45.403	39.104	36.949	1.00 45.90
ATOM	2174	N		C1107	48.527	35.962	35.531	1.00 42.56
ATOM	2175	CA		C1107	49.593	34.961	35.679	1.00 44.02
ATOM	2176	C		C1107	50.420	35.168	36.946	1.00 46.86
ATOM	2177	0		C1107	50.888	36.295	37.127	1.00 49.56
ATOM	2178	CB		C1107	50.539	34.986	34.483	1.00 38.92
ATOM	2179	CG		C1107	49.970	34.778	33.106	1.00 37.89
ATOM	2180	CD1		C1107	51.073	34.991	32.082	1.00 39.13
ATOM	2181	CD2		C1107	49.400	33.350	32.925	1.00 34.26
ATOM	2182	34		C1108	50.605	34.176	37.803	1.00 49.68
ATOM	2183	CA		C1108	51.362	34.337	39.032	1.00 53.06
ATOM	2184	C		C1108	52.666	33.527	38.953	1.00 51.34
ATOM	2185	0		C1108	53.677	34.091	38.558	1.00 52.57
ATOM	2186	CB		C1108	50.645	33.861	40.328	1.00 54.61
ATOM	2187	CG		C1108	49.538	34.857	40.622	1.00 56.02
ATOM	2188	CD1		C1108	48.208	34.511	40.387	1.00 56.47
ATOM	2189	CD2	TYR	C1108	49.864	36.137	41.055	1.00 56.41
MOTA	2190	CE1	TYR	C1108	47.207	35.441	40.597	1.00 56.50
ATOM	2191	CE2	TYR	C1108	48.864	37.072	41.271	1.00 57.46
MOTA	2192	CZ	TYR	C1108	47.544	36.698	41.044	1.00 57.18
ATOM	2193	OH		C1108	46.577	37.639	41.267	1.00 58.64
ATOM	2194	N	GLU	C1109	52.585	32.293	39.382	1.00 50.07
MOTA	2195	CA	GLU	C1109	53.718	31.412	39.346	1.00 50.65
MOTA	2196	C	GLU	C1109	53.548	30.323	38.275	1.00 48.97
ATOM	2197	0	GLU	C1109	54.587	29.965	37.719	1.00 47.87
MOTA	2198	CB	GLU	C1109	53.958	30.616	40.626	1.00 53.87
ATOM	2199	CG	GLU	C1109	53.835	31.284	41.965	1.00 58.53
MOTA	2200	CD	GLU	C1109	54.896	32.352	42.202	1.00 60.45
ATOM	2201	OE1	GLU	C1109	56.092	31.991	42.113	1.00 61.68
ATOM	2202	OE2	GLU	C1109	54.482	33.514	42.480	1.00 61.69
ATOM	2203	N	LYS	C1110	52.345	29.727	38.224	1.00 47.13
MOTA	2204	CA	LYS	C1110	52.186	28.577	37.324	1.00 45.74
ATOM	2205	C	LYS	C1110	50.816	28.638	36.645	1.00 42.35
ATOM	2206	0	LYS	C1110	49.924	29.188	37.270	1.00 41.09
ATOM	2207	CB	LYS	C1110	52.400	27.320	38.151	1.00 48.67
ATOM	2208	CG	LYS	C1110	52.564	26.005	37.440	1.00 53.26
ATOM	2209	CD	LYS	C1110	53.174	24.877	38.287	1.00 56.04
ATOM	2210	CE	LYS	C1110	54.685	25.087	38.489	1.00 58.45
ATOM	2211	NZ	LYS	C1110	55.447	23.870	38.929	1.00 58.97
ATOM	2212	N	PHE	C1111	50.666	28.295	35.359	1.00 37.18
MOTA	2213	CA		C1111	49.325	28.434	34.823	1.00 36.07
MOTA	2214	C		C1111	49.163	27.464	33.658	1.00 33.65
ATOM	2215	0		C1111	49.926	27.605	32.736	1.00 31.39
ATOM	2216	CB		C1111	48.962	29.880	34.438	1.00 36.60
ATOM	2217	CG	PHE	C1111	47.531	30.157	34.143	1.00 37.58

ATOM	2218	CD1	PHE	C1111	4 6	.754	30.	911	35.	026	1.00	40.75
ATOM	2219	CD2	PHE	C1111	4 6	.914	29.	636	33.	009	1.00	37.53
ATOM	2220	CEL	PHE	C1111	4.5	.395	31.	140	34.	795	1.00	40.10
ATOM	2221	CE2		C1111		.582	29.			758	1.00	37.72
ATOM	2222	CZ		C1111		. 824	30.			643	1.00	38.68
ATOM	2223	N		C1112		.115	26.			719	1.00	28.79
ATOM	2224	CA		C1112		.688	25.			634	1.00	31.45
		C		C1112		.183	26.			377		30.94
ATOM	2225									377	1.00	
ATOM	2226	0		C1112		.468	26.					29.01
MOTA	2227	CB		C1112		.744	24.			099	1.00	32.34
ATOM	2228	OG1		C1112		.026	24.			723	1.00	35.99
ATOM	2229	CG2		C1112		.738	23.			909		32.22
ATOM	2230	N		C1113		.708	26.			158	1.00	28.73
ATOM	2231	CA		C1113		.309	26.			840		28.29
ATOM	2232	С	TYR	C1113		.709	24.			942	1.00	31.34
ATOM	2233	0	TYR	C1113	44	.388	23.	615	30.	928		25.50
ATOM	2234	CB	TYR	C1113	4.4	.203	26.	353	29.	330	1.00	27.79
ATOM	2235	CG	TYR	C1113	4.4	. 656	27.	778	29.	016	1.00	29.11
ATOM	2236	CDl	TYR	C1113	4.5	.753	27.	954	28.	181	1.00	30.15
ATOM	2237	CD2	TYR	C1113	44	.032	28.	897	29.	544	1.00	27.99
ATOM	2238	CE1	TYR	C1113	4.6	.199	29.	241	27.	868	1.00	31.57
ATOM	2239	CE2		C1113		.460	30.			201	1.00	30.17
ATOM	2240	CZ		C1113		.571	30.			371	1.00	30.26
ATOM	2241	OH		C1113		.068	31.			045	1.00	30.20
ATOM	2242	N		C1114		.398	24.			120		29.12
ATOM	2243	CA		C1114		. 638	23.			035	1.00	30.29
ATOM	2244	C		C1114		882	22.			625	1.00	30.26
ATOM	2245	0		C1114		791	23.			680		30.70
ATOM	2245	СВ		C1114		1.127		678		199	1.00	
				C1114		2.135	21.			515		28.43
ATOM ATOM	2247	N CA				3.371	21.			199		30.36
	2248			C1115								34.03
ATOM	2249	C		C1115		1.138		933		334		
ATOM	2250	0		C1115		9.913	20.			653		35.50
MOTA	2251	N		C1116		1.445		017		046		35.79
MOTA	2252	CA		C1116		.554		877		918		41.16
ATOM	2253	C		C1116		.987		601		199		48.93
ATOM	2254	CB		C1116		.660		990		877		40.53
ATOM	2255	CGI		C1116		332		381		419		39.34
MOTA	2256	CG2		C1116		9.797		709		629		40.56
MOTA	2257	CD1		C1116		.844		462		474		39.48
MOTA	2258	N	ASP	C1117	4 (0.096	18.	690	23.	816		56.34
ATOM	2259	CA		C1117	4 (0.671	17.	809	22.	759	1.00	64.41
ATOM	2260	C	ASP	C1117	3.9	9.582	17.	226	21.	862	1.00	67.05
ATOM	2261	0	ASP	C1117	3.8	3.632	16.	639	22.	384	1.00	66.11
ATOM	2262	CB	ASP	C1117	4:	1.552	16.	679	23.	243	1.00	66.12
ATOM	2263	CG	ASP	C1117	42	2.980	17.	054	23.	608	1.00	68.11
ATOM	2264	OD1	ASP	C1117	43	3.730	17.	676	22.	830	1.00	69.52
ATOM	2265	OD2	ASP	C1117	43	3.216	16.	706	24.	787	1.00	68.31
ATOM	2266	N	CYS	C1118	3 :	9.775	17.	421	20.	548	1.00	71.27
ATOM	2267	CA		C1118		3.800		948		563	1.00	75.06
ATOM	2268	C		C1118		9.057		522		165	1.00	
ATOM	2269	CB		C1118		7.387		351		997		74.91
ATOM	2270	N		C1119		3.094		334		244		81.20
ATOM	2271	CA		C1119		3.055		960		924	1.00	
ATOM	2272	C		C1119		7.335		232		.787		84.56
ATOM	2273	0		C1119		7.930		898		.740		85.44
ATOM	2274	CB		C1119		9.493		300		.476		83.21
ATON	4414	CD	DEK	CTTT3	3	2.433	TO.	200	13	. 1 / 0	1.00	03.21

ATOM	2275	N	21.2	C11:	2.0	36.028	16.990	14.863	3 00	85.16
ATOM	2276	CA		C11:		35.171	16.384	13.874		84.89
ATOM	2277	C		C11:		34.722	14.957	14.213		85.19
ATOM	2278	0		C11:		33.876	14.494	13.396		85.38
ATOM	2279	CB		C11:		35.714	16.345	12.447		84.84
TER	2215	CD	ALDA	CII.	20	22.,14	10.545	12.447	2.00	04.02
HETATM	2280	Cl	IN3	D	1	27.737	34.907	12.224	1 00	40.84
HETATM		N2	INS		1	28.220	33.661	12.185		40.67
HETATM		C3	INS		î	27.362	32.629	12.233		40.61
HETATM		C4	IN3		1	25.970	32.787	12.233		41.94
HETATM		C5	IN3		î	25.570	34.130	12.362		41.03
HETATM		Ne	INS		î	26.428	35.160	12.315		40.65
HETATM		N8	IN3	D	1	27.727	31.299	12.203		42.23
HETATM		C9		D	1	26.517	30.664	12.312		42.50
HETATM		C10			1	25.373	31.506	12.312		44.61
HETATM		N12	INB		1	24.231	34.490	12.467		43.99
HETATM		C13	INB		1	23.982	30.977	12.436		43.99
HETATM		C14	INS		1	29.096	30.727	12.430		42.52
HETATM		C15	IN3		1					
HETATM		C16	INS	D	1	22.960	31.497	13.194		50.46
HETATM		C17	INS		1	21.667	29.804			
HETATM		C18	INS	D	1	22.357	29.258	12.531		51.31
HETATM			INS		1			11.751		51.58
HETATM						23.637	29.839	11.712		51.00
		N23	IN3		1	20.099	29.245	12.581		52.79
HETATM		S24	IN3		1	19.137	29.209	13.847		53.21
HETATM		025	IN3		1	19.809	29.557	15.058		54.86
HETATM		026	IN3		1	18.402	27.997	13.940		52.02
		C27	IN3		1	17.984	30.563	13.554		59.14
HETATM		C28	IN3		1	17.058	30.565	12.515		62.44
HETATM		C29	IN3		1	16.171	31.631	12.344		63.41
HETATM			IN3		1	16.219	32.721	13.201		61.99
HETATM		C31	INB		1	17.146	32.728	14.233		61.19
		C32	IN3		1	18.012	31.655	14.412		59.69
HETATM			IN3		1	17.000	29.190	11.437		72.20
HETATM			IN3		1	14.971	31.634	11.070		66.32
HETATM		F38	IN3		1	22.188	28.164	10.970		50.23
HETATM		C39	IN3		1	29.429	30.465	13.689		41.55
HETATM			IN3	D	1	30.719	29.713	13.975		41.76
HETATM		C41	IN3		1	30.922	28.491	13.060		42.34
HETATM			IN3		1	30.611	28.800	11.579		44.10
HETATM		C43	IN3		1	29.231	29.447	11.376		43.74
		C52	IN3		1	32.457	27.054	14.408		40.98
HETATM		C53	IN3		1	33.702	26.161	14.218		39.93
HETATM		N54	IN3		1	34.865	27.024	14.047		40.92
HETATM		C55	IN3	D	1	34.719	27.865	12.858		41.55
HETATM		C56		D	1	33.437	28.707	12.946		41.49
HETATM		N57	IN3	D	1	32.249	27.891	13.211		41.23
HETATM	2346	C67	INB	D	1	36.230	26.430	14.126	1.00	38.95
TER		_								
ATOM	2355	0	HOH		1	31.108	33.861	12.284		32.88
ATOM	2356	0	HOH		2	26.872	17.118	31.780		27.53
ATOM	2357	0	HOH		3	33.552	31.769	15.218		24.69
ATOM	2358	0	HOH		4	47.567	25.314	28.603		31.73
MOTA	2359	0	HOH		5	2.429	17.063	30.925		30.32
MOTA	2360	0	HOH		7	33.908	23.176	25.246		32.79
ATOM	2361	0	HOH		8	16.942	20.674	27.837		29.27
ATOM	2362	0	HOH	W	9	41.194	27.270	31.243	1.00	27.50

					0.6.000			
MOTA	2363	0	HOH W	10	36.797	18.417	32.828	1.00 30.03
ATOM	2364	0	HOH W	11	28.851	18.044	20.371	1.00 31.02
ATOM	2365 2366	0	HOH W	12	15.509 9.416	22.554	31.309	1.00 36.36
ATOM		0			24.583	41.060	16.124	1.00 34.74
ATOM ATOM	2367 2368	0	HOH W	14	7.357	41.316	15.797	1.00 44.69
ATOM	2369	0	HOH W	16	40.089	39.018	35.286	1.00 43.58
ATOM	2370	c	HOH W	17	42.573	39.050	31.498	1.00 33.36
ATOM	2371	ő	HOH W	18	18.935	40.500	18.279	1.00 34.03
ATOM	2372	0	HOH W	19	13.481	27.068	41.482	1.00 45.27
ATOM	2373	ō	HOH W	20	19.798	23.284	27.046	1.00 32.39
ATOM	2374	ō	HOH W	22	13.750	26.546	29.238	1.00 33.61
ATOM	2375	ō	HOE W	23	15.599	37.531	37.224	1.00 41.73
ATOM	2376	0	HOH W	24	45.162	20.392	30.028	1.00 51.51
ATOM	2377	0	HOH W	25	33.164	26.427	17.812	1.00 30.96
ATOM	2378	0	HOH W	27	25.096	40.967	30.617	1.00 31.07
ATOM	2379	0	HOH W	28	44.306	23.553	33.708	1.00 44.45
MOTA	2380	0	HOH W	29	14.071	17.249	33.601	1.00 32.43
MOTA	2381	0	W HOH	30	30.157	24.039	23.053	1.00 31.23
ATOM	2382	0	HOH W	31	21.111	43.623	15.597	1.00 74.93
MOTA	2383	0	HOH W	33	19.327	17.632	28.859	1.00 33.09
MOTA	2384	0	HOH W	34	13.241	23.665	39.267	1.00 41.89
MOTA	2385	0	HOH W	35	31.519	44.776	18.549	1.00 43.36
MOTA	2386	0	HOH W	36	34.470	39.819	38.307	1.00 52.30
MOTA	2387	0	HOH M	37	19.740	20.765	27.651	1.00 65.54
MOTA	2388	0	HOH W	38	44.917	36.546	20.426	1.00 59.90
ATOM	2389	0	HOH W	40	17.011	9.839	35.866	1.00 47.22
MOTA	2390	0	HCH W	41	38.945	20.370	30.087	1.00 25.50
ATOM	2391	0	HOH W	43	46.179	22.872	28.085	1.00 39.76
ATOM	2392	0	HOH W	44	33.414	46.650	18.569	1.00 52.18
ATOM	2393	0	HOH W	45	25.781	19.393	41.795	1.00 39.77
ATOM ATOM	2394	0	HOH W	46 47	25.879 12.674	14.880 31.920	30.825 35.287	1.00 26.83
ATOM	2395	0	HOH W	4.8	36.038	20.519	22.613	1.00 41.22
ATOM	2397	0	HOH W	49	9.232	35.876	28.692	1.00 40.75
ATOM	2398	0	HOH W	50	36.218	20.561	20.320	1.00 40.50
ATOM	2399	Ö	HOH W	54	27.796	43.597	11.505	1.00 56.18
ATOM	2400	o	HOH W	56	43.257	28.114	21.417	1.00 40.56
ATOM	2401	ō	HOH W	57	42.324	44.229	29.443	1.00 56.40
ATOM	2402	ō	HOH W	58	31.439	22.023	21.413	1.00 32.43
ATOM	2403	Ö	HOH W	59	49.313	32.007	37.867	1.00 46.71
ATOM	2404	0	HOH W	60	14.875	35.132	15.522	1.00 39.98
ATOM	. 2405	0	HOH W	62	20.722	5.005	29.475	1.00 39.73
ATOM	2406	0	HOH W	63	45.974	43.256	29.290	1.00 41.18
ATOM	2407	0	HOH W	64	42.241	38.248	37.028	1.00 43.70
ATOM	2408	0	HOH W	65	32.550	42.002	39.832	1.00 36.99
ATOM	2409	0	W HOH	67	39.110	46.531	21.311	1.00 37.71
ATOM	2410	0	HOH W	68	24.108	20.905	21.953	1.00 53.77
ATOM	2411	0	HOH W	69	1.460	21.994	31.199	1.00 37.30
MOTA	2412	0	HOH W	70	49.466	21.211	34.770	1.00 51.34
ATOM	2413	0	HOH W	71	36.003	21.023	42.825	1.00 40.91
ATOM	2414	0	HOH W	73	22.188	25.684	4.901	1.00 54.10
ATOM	2415	0	HOH W	74	39.079	46.157	42.492	1.00 62.53
ATOM	2416	0	HOH W	75	40.067	30.895	33.482	1.00 47.79
ATOM	2417	0	HOH W	76	46.668	20.370	34.397	1.00 41.58
ATOM	2418	0	HOH W	78	11.682	32.018	39.657	1.00 44.53

20.567 30.929 42.014 1.00 56.17

ATOM	2420	0	HOH W	80	22.313	16.019	43.949	1.00	47.96
ATOM	2421	0	HOH W	83	33.379	32.767	48.175	1.00	44.70
ATOM	2422	0	HOH W	84	28.448	47.110	11.329		72.32
ATOM	2423	0	HOH W	85	11.988	40.527	14.366	1.00	57.96
ATOM	2424	0	HOH W	86	11.100	37.338	30.951		55.75
ATOM	2425	ō	HOH W	87	32,424	25.662	10.927		60.85
ATOM	2426	0	HOH W	88	40.553	21.024	36.981		56.71
ATOM	2427	0	HOH W	89	20.806	40.663	41.692		49.92
ATOM	2428	0	HOH W	90	23.126	21.071			
							24.679		28.98
ATOM	2429	0	HOH W	91	21.847	27.668	22.076		39.04
ATOM	2430	0	HOH W	92	17.442	12.682	22.568		42.46
MOTA	2431	0	HOH W	94	10.365	22.725	38.862		42.24
ATOM	2432	0	HOH W	96	12.915	13.110	35.504		43.57
ATOM	2433	0	HOH W	97	11.437	18.561	35.709		49.64
ATOM	2434	0	HOH W	98	18.202	17.009	21.807	1.00	60.40
ATOM	2435	0	HOH W	99	13.090	22.057	22.029	1.00	44.65
ATOM	2436	0	HOH W	100	13.782	3.003	30.101	1.00	45.94
ATOM	2437	0	HOH W	101	37.114	30.510	14.091	1.00	54.40
ATOM	2438	0	HOH W	102	39.281	19.995	32.505	1.00	38.67
ATOM	2439	0	HOH W	103	19.163	41.538	33.907	1.00	49.16
ATOM	2440	0	HOH W	105	8.161	24.650	30.444		38.87
ATOM	2441	ō	HOH W	106	19.044	34.146	43.247		36.17
ATOM	2442	ō	HOH W	107	52.411	29.944	20.957		47.78
ATOM	2443	0	HOH W	109	40.926	37.945	21.207		57.61
ATOM	2444	0	HOH W	110	23.910	22.805			
ATOM	2445	0	HOH W	111		43.384	45.525		56.43
ATOM					23.876		19.810		29.77
	2446	0	HOH W	112	6.751	36.672	21.579		62.88
ATOM	2447	0	HOH W	113	43.463	27.806	35.372		49.32
ATOM	244B	0	HOH W	114	33.230	32.283	12.794		37.37
ATOM	2449	0	HOH W	115	39.120	18.996	40.839		82.49
MOTA	2450	0		116	17.786	13.772	37.357	1.00	49.91
ATOM	2451	0	HOH W	117	20.655	9.465	38.822	1.00	43.82
ATOM	2452	0	HOH W	118	7.544	39.794	24.678	1.00	56.43
ATOM	2453	0	HOH W	119	34.363	21.476	9.358	1.00	64.39
ATOM	2454	0	HOH W	120	14.923	37.925	31.147	1.00	51.98
ATOM	2455	0	HOH W	121	14.386	25.644	36.407	1.00	47.28
ATOM	2456	0	HOH W	122	33.578	21.114	23.402	1.00	36.98
ATOM	2457	0	HOH W	123	42.616	19.765	31.993	1.00	46.67
ATOM	2458	0	HOH W	124	0.324	31.122	29.775		85.67
ATOM	2459	0		125	44.223	21.073	33.792		58.84
ATOM	2460	ō	HOH W		13.220	29.507	33.957		42.26
ATOM	2461	0	HOH W	127	24.661	6.250	44.308		53.58
ATOM	2462	ō	HOH W	130	37.555	26.025	18.301		50.21
ATOM	2463	0	HOH W	131	29.409	15.521	23.790		37.37
ATOM	2464	Ö	HOH W	134	37.198	41.960	35.518		40.19
ATOM	2465	0	HOH W						
ATOM	2466	0	HOH W	135	38.741	36.516	21.186		31.33
					20.039	45.048	11.998		67.09
ATOM	2467	0	HOH W	137	44.865	39.383	33.992		42.87
ATOM	2468	0	HOH W	138	47.499	41.543	34.693		41.95
ATOM	2469	0	HOH W	139	14.470	39.588	29.214		39.88
ATOM	2470	0	HOH W	140	25.148	21.128	18.186		55.16
ATOM	2471	0		141	19.506	9.850	24.839		56.90
ATOM	2472	0	HOH W	142	39.082	7.569	29.845		50.85
ATOM	2473	0		143	37.915	8.580	37.497	1.00	73.18
ATOM	2474	0	HOH W	144	37.234	11.075	36.059	1.00	55.17
ATOM	2475	0		145	18.909	16.767	43.975	1.00	45.07
ATOM	2476	0	HOH W	146	53.564	36.062	20.842	1.00	35.39

Docket/App No.: 2079.1037-001

Title: Method of Identifying Inhibitors of TIE-2
Inventors: Nancy J. Bump et al.

ATOM 2477 O HOH W 147 TER

21.172 42.848 12.347 1.00 52.85

DECM	2							
ATOM ATOM	1	13		A 818	77.717	45.877	1.677	1.00100.00
ATOM	2	CA		A 818	76.698	46.966	1.561	1.00100.00
ATOM	3			A 818	75.278	46.411	1.674	1.00100.00
ATOM	5	CB	YAL I		74.803	46.162	2.781	1.00100.00
			VAL 2		76.875	47.697	0.239	1.00 68.23
ATOM	9	N	LEU A		74.617	46.228	0.530	1.00100.00
ATOM ATOM	10	CA		4 819	73.248	45.707	0.456	1.00100.00
	11	C	LEU 2		72.629	45.997	-0.918	1.00100.00
ATOM	12	0	LEU /		71.622	46.589	-1.003	1.00100.00
ATOM	13	CB	LEU A		72.369	46.345	1.536	1.00100.00
ATOM	14	CG	LEU /		70.873	46.053	1,525	1.00100.00
ATOM	1.5	CD1			70.592	44.975	2.511	1.00100.00
ATOM	16	CD2	LEU A		70.078	47.283	1.865	1.00100.00
ATOM	18	N	ASP A		73.234	45.474	-1.984	1.00100.00
ATOM	19	CA	ASP A		72.753	45.676	-3.359	1.00100.00
ATOM	20	C		820	71.292	46.104	-3.464	1.00100.00
ATOM	21	0	ASP A		70.399	45.421	-2.983	1.00100.00
ATOM	22	CB	ASP A		72.969	44.396	-4.177	1.00 99.21
ATOM	23	CG	ASP A		71.872	44.160	-5.218	1.00 99.21
ATOM	24		ASP A		71.584	42.982	-5.509	1.00 99.21
ATOM	25	OD2		820	71.303	45.140	-5.750	1.00 99.21
ATOM	27	N		821	71.050	47.227	-4.126	1.00 93.11
MOTA	28	CA	TRP A		69.694	47.719	-4.268	1.00 93.11
MOTA	29	C	TRP 7		68.716	46.617	-4.650	1.00 93.11
ATOM	30	0		821	€7.904	46.199	-3.849	1.00 93.11
ATOM	31	CB	TRP 2		69.639	48.863	-5.283	1.00 97.87
ATOM	3.2	CG	TRP A		68.703	49.927	-4.847	1.00 97.87
ATOM	33	CD1		821	68.605	50.452	-3.597	1.00 97.87
ATOM	34	CD2		821	67.667	50.542	-5.622	1.00 97.87
ATOM	3.5	NEl	TRP A		67.567	51.352	-3.537	1.00 97.87
ATOM	36	CE2	TRP A		66.974	51.429	-4.766	1.00 97.87
ATOM	37	CE3	TRP A		67.255	50.429	-6.949	1.00 97.87
ATOM	38	CZ2	TRP A		65.897	52.197	-5.193	1.00 97.87
ATOM	3.9	CZ3		821	66.180	51.192	-7.374	1.00 97.87
ATOM	40	CH2	TRP A		65.512	52.065	-6.496	1.00 97.87
ATOM	43	N	ASN A		68.798	46.140	-5.896	1.00100.00
ATOM	44	CA	ASN A		67.901	45.077	-6.364	1.00100.00
ATOM	45	С	ASN A		67.686	43.985	-5.314	1.00100.00
ATOM	46	0	ASN A		66.545	43.614	-5.030	1.00100.00
ATOM	47	CB	ASN A		68.462	44.410	-7.624	1.00 56.29
ATOM	48	CG	ASN A		68.707	42.917	-7.427	1.00 56.29
ATOM	49	OD1	ASN A		69.755	42.499	-6.902	1.00 56.29
ATOM	50	ND2	ASN A		67.739	42.114	-7.837	1.00 56.29
ATOM	54	N	ASP A		68.799	43.469	-4.776	1.00 99.96
ATOM	55	CA	ASP A		68.825	42.413	-3.756	1.00 99.96
ATOM	56	C	ASP A		67.823	42.654	-2.650	1.00 99.96
ATOM	57	0	ASP A		67.545	41.765	-1.846	1.00 99.96
ATOM	58	CB	ASP A		70.218	42.308	~3.153	1.00100.00
ATOM	60	N	ILE A		67.303	43.875	-2.605	1.00 80.08
ATOM	61	CA	ILE A		66.315	44.270	-1.616	1.00 80.08
ATOM	62	C	ILE A		64.958	44.392	-2.274	1.00 80.08
ATOM	63	0	ILE A		64.703	45.359	-2.973	1.00 80.08
ATOM	64	CB	ILE A		66.651	45.641	-0.992	1.00100.00
ATOM	65	CG1	ILE A		67.806	45.506	0.009	1.00100.00
ATOM	66	CG2	ILE A		65.417	46.206	-0.307	1.00100.00
ATOM	67	CD1	ILE A	824	69.048	44.906	-0.577	1.00100.00

Market

ATOM	69	N	LYS	. 8	25	64.098	43.404	-2.036	1.00 99.67
ATOM	7.0	CA	LYS A			62.735	43.391	-2.580	1.00 99.67
ATOM	71	C		4 8		61.938	44.544	-1.938	1.00 99.67
ATOM	72	ō		4 8		61.130	44.334	-1.027	1.00 99.67
ATOM	73	CB	LYS 2			62.056	42.021	-2.286	1.00 63.59
ATOM	75	N	PHE			62.171	45.762	-2.420	1.00 69.32
ATOM	76	CA	PHE			61.502	46.933	-1.875	1.00 69.32
ATOM	77	C		. 8		59.977	46.823	-1.994	1.00 69.32
ATOM	78	Ö	PHE I			59.500	45.922	-2.684	1.00 69.32
ATOM	79	CB	PHE A			62.060	48.158	-2.587	1.00 99.11
ATOM	80	CG		3 8		63.558	48.351	-2.376	1.00 99.11
ATOM	81	CD1	PHE I			64.470	47.961	-3.343	1.00 99.11
ATOM		CD2		4 8 4 8		64.045	48.959	-1.215	1.00 99.11
	82		PHE I					-3.157	1.00 99.11
ATOM	83	CEl				65.839	48.178		
ATOM	84	CE2		4 8		65.418	49.179	-1.027	1.00 99.11
ATOM	85	CZ	PHE :			66.307	48.791	-1.995 -1.307	
ATOM	87	N	GLN :			59.222	47.691		
ATOM	88	CA	GLN .			57.728	47.659	-1.347	1.00 70.60
ATOM	89	C	GLN .		_	57.010	49.023	-1.173	1.00 70.60
ATOM	90	0	GLN .			57.401	49.946	-1.874	1.00 70.60
ATOM	91	CB	GLN .			57.178	46.624	-0.337	1.00100.00
MOTA	92	CG	GLN .			57.627	45.151	-0.598	1.00100.00
ATOM	93	CD	GLN .			56.797	44.413	-1.665	1.00100.00
ATOM	94	OE1	GLN .			55.642	44.036	-1.433	1.00100.00
MOTA	95	NE2	GLN .			57.396	44.196	-2.831	1.00100.00
MOTA	99	N	ASP .	8 4	328	56.000	49.149	-0.278	1.00 99.97
ATOM	100	CA	ASP .	8 4	328	55.218	50.418	-0.055	1.00 99.97
ATOM	101	C	ASP .	8 A	328	55.490	51.355	1.163	1.00 99.97
ATOM	102	0	ASP .	9	328	56.284	51.045	2.038	1.00 99.97
ATOM	103	CB	ASP .	8 A	328	53.723	50.128	0.010	1.00100.00
ATOM	104	CG	ASP .			53.034	50.839	1.214	1.00100.00
ATOM	105	OD1	ASP .	A 8	328	52.702	52.037	1.109	1.00100.00
ATOM	106	OD2	ASP .			52.834	50.215	2.280	1.00100.00
ATOM	108	N	VAL .	8 A	329	54.787	52.494	1.212	1.00100.00
MOTA	109	CA	VAL .	A 8	329	54.900	53.488	2.295	1.00100.00
MOTA	110	C	VAL .			54.384	53.014	3.639	1.00100.00
ATOM	111	0	VAL .			53.683	52.012	3.703	1.00100.00
ATOM	112	CB	VAL .	A 8	329	54.162	54.786	1.912	1.00100.00
MOTA	114	N	ILE .	3 A	330	54.726	53.770	4.695	1.00 76.50
MOTA	115	CA	ILE			54.342	53.500	6.102	1.00 76.50
MOTA	116	C	ILE			53.685	54.717	6.782	1.00 76.50
ATOM	117	0	ILE		330	52.464	54.830	6.808	1.00 76.50
MOTA	118	CB			330	55.571	53.069	6.979	1.00 83.02
MOTA	119	CGl	ILE	Α ε	330	55.888	51.607	6.755	1.00 83.02
ATOM	120	CG2	ILE	Aε	330	55.269	53.185	8.437	1.00 83.02
ATOM	121	CD1	ILE			57.118	51.163	7.437	1.00 83.02
MOTA	123	N	GLY	Α ε	331	54.492	55.626	7.327	1.00100.00
ATOM	124	CA	GLY			53.930	56.779	8.009	1.00100.00
ATOM	125	C	GLY			54.664	58.090	7.811	1.00100.00
ATOM	126	0	GLY			54.659	58.963	8.677	1.00100.00
MOTA	128	N	GLU	Aξ	332	55.301	58.216	6.660	1.00 46.31
ATOM	129	CA	GLU			56.045	59.418	6.271	1.00 46.31
ATOM	130	C	GLU	Aξ	B32	57.586	59.215	6.265	1.00 46.31
ATOM	131	0	GLU	Aε	832	58.101	58.149	5.892	1.00 46.31
ATOM	132	CB	GLU	Aε	832	55.668	60.618	7.158	1.00100.00
ATOM	133	CG	GLU	Α 8	832	54.587	61.531	6.557	1.00100.00
ATOM	134	CD	GLU	A 8	832	54.197	62.702	7.473	1.00100.00

ATOM	135	OE1	GLU	Δ	832	52.980	62.942	7.660	1.00100.00
ATOM	136	OE2	GLU		832	55.107	63.387	8.002	1.00100.00
ATOM	138	N	GLY		833	58,330	60.239	6.650	1.00100.00
ATOM	139	CA	GLY			59.762	60.092	6.672	1.00100.00
ATOM	140	C	GLY			60.311	61.410	7.090	1.00100.00
ATOM	141	0	GLY			60.675	61.601	8.251	1.00100.00
ATOM	143	N	ASN			60.339	62.327	6.130	1.00 87.28
ATOM	144	CA	ASN			60.829	63.680	6.360	1.00 87.28
		C	ASN			62.306	63.520	6.539	1.00 87.28
ATOM	145	0	ASN		834	62.684	62.859	7.613	1.00 87.28
ATOM	146 147	CB	ASN			60.114	64.306	7.570	1.00100.00
ATOM		CG	ASN			60.641	65.685	7.932	1.00100.00
ATOM	148		ASN				65.865	8.248	1.00100.00
ATOM	149	OD1				61.822		7.903	1.00100.00
ATOM	150	ND2	ASN			59.751	66.671	5.782	1.00100.00
ATOM	154	N	PHE			63.131	64.125		
ATOM	155	CA	PHE		835	64.561	64.036	5.925	1.00 68.16
ATOM	156	C	PHE		835	64.700	62.693	6.578	1.00 68.16
ATOM	157	0	PHE			65.138	62.586	7.733	1.00 68.16
ATOM	158	CB	PHE			65.073	65.139	6.840	1.00 80.78
MOTA	159	CG			835	65.317	66.447	6.135	1.00 80.78
ATOM	160	CD1	PHE			64.950	67.651	6.733	1.00 80.78
MCTA	161	CD2	PHE			65.931	66.475	4.877	1.00 80.78
ATOM	162	CE1	PHE		835	65.190	68.856	6.097	1.00 80.78
ATOM	163	CE2	PHE			66.178	67.689	4.226	1.00 80.78
ATOM	164	CZ	PHE		835	65.805	68.881	4.838	1.00 80.78
ATOM	166	N	GLY	Α	836	64.226	61.691	5.832	1.00100.00
ATOM	167	CA	GLY			64.252	60.304	6.257	1.00100.00
ATOM	168	C	GLY		836	62.962	59.578	5.914	1.00100.00
ATOM	169	0	GLY			62.314	59.012	6.792	1.00100.00
ATOM	171	N	GLN		837	62.599	59.565	4.636	1.00 88.37
ATOM	172	CA	GLN	Α	837	61.356	58.915	4.214	1.00 88.37
ATOM	173	С	GLN	Α	837	61.114	57.472	4.701	1.00 88.37
ATOM	174	0	GLN	А	837	61.739	56.544	4.186	1.00 88.37
ATOM	175	CB	GLN	Α	837	61.206	58.983	2.666	1.00 70.59
ATOM	176	CG	GLN	Α	837	62.424	58.531	1.876	1.00 70.59
ATOM	177	CD	GLN	Α	837	62.484	59.097	0.437	1.00 70.59
ATOM	178	OE1	GLN	A.	837	63.560	59.517	-0.041	1.00 70.59
ATOM	179	NE2	GLN	Α	837	61.327	59.088	-0.263	1.00 70.59
MOTA	183	N	VAL	A	838	60.211	57.302	5.687	1.00 63.61
ATOM	184	CA	VAL	Α	838	59.835	55.959	6.213	1.00 63.61
ATOM	185	C	VAL	Α	838	58.710	55.222	5.481	1.00 63.61
ATOM	186	0	VAL	Α	838	57.525	55.380	5.807	1.00 63.61
ATOM	187	CB	VAL	Α	838	59.384	55.939	7.692	1.00 61.77
ATOM	188	CG1	VAL	A	838	60.243	54.967	8.446	1.00 61.77
ATOM	189	CG2	VAL	Α	838	59.418	57.290	8.292	1.00 61.77
ATOM	191	N	LEU	Α	839	59.114	54.397	4.520	1.00100.00
ATOM	192	CA	LEU	A	839	58.201	53.584	3.738	1.00100.00
ATOM	193	C	LEU	A	839	58.399	52.107	4.098	1.00100.00
ATOM	194	ō	LEU		839	59.473	51.694	4.507	1.00100.00
ATOM	195	CB	LEU		839	58.464	53.783	2.244	1.00100.00
ATOM	196	CG	LEU		839	58.836	55.168	1.719	1.00100.00
ATOM	197	CD1	LEU		839	58.069	56.233	2.461	1.00100.00
ATOM	198	CD2	LEU			60.323	55.367	1.853	1.00100.00
ATOM	200	N		A	840	57.352	51.315	3.969	1.00 58.16
ATOM	201	CA	LYS	A	840	57.459	49.901	4.259	1.00 58.16
ATOM	202	C	LYS			58.091	49.174	3.081	1.00 58.16
ATOM	202	0	LYS			57.837	49.497	1.943	1.00 58.16
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Inventors:

Title: Method of Identifying Inhibitors of TIE-2 Nancy J. Bump et al.

204 CB LYS A 840 56.071 49.313 4.549 1.00 67.71 ATOM ATOM 205 CG LYS A 840 56.075 47.809 4.810 1.00 67.71 55.274 47.391 55.467 45.926 56.848 45.463 6.047 1.00 67.71 206 CD ATOM LYS A 840 207 CE LYS A 840 208 NZ LYS A 840 6.360 1.00 67.71 ATOM 6.017 1.00 67.71 MOTA 213 N. ALA A 841 58.916 48.176 3.344 1.00 99.75 MOTA 214 CA ALA A 841 ATOM 59.514 47.452 2.241 1.00 99.75 215 C ALA A 841 59.845 46.037 2.620 1.00 99.75 ATOM 216 O ALA A 841 59.830 45.684 3.796 1.00 99.75 MOTA 60.748 48.152 ATOM 217 CB ALA A 841 1.771 1.00 78.22 60.143 45.231 1.605 1.00100.00 MOTA 219 N ARG A 842 ATOM 220 CA ARG A 842 60.499 43.832 1.798 1.00100.00 221 C ARG A 842 61.972 43.576 1.429 1.00100.00 ATOM ATOM 222 O ARG A 842 62.288 43.082 0.352 1.00100.00 223 CB ARG A 842 59.574 42.951 0.973 1.00100.00 ATOM 225 N ATOM ILE A 843 62.868 43.919 2.348 1.00100.00 226 CA ILE A 843 64.301 43.743 I.148 1.00100.00 MOTA ATOM 227 C ILE A 843 64.642 42.262 2.174 1.00100.00 228 0 63.952 41.488 2.844 1.00100.00 ATOM ILE A 843 229 CB ILE A 843 229 CB ILE A 843 230 CGI ILE A 843 231 CG2 ILE A 843 232 CD1 ILE A 843 234 N LYS A 844 65.094 44.489 3.263 1.00 99.77 ATOM 65.193 45.960 66.487 43.937 2.907 1.00 99.77 ATOM 3.421 1.00 99.77 ATOM 2.554 1.00 99.77 1.435 1.00 77.20 1.379 1.00 77.20 ATOM 63.857 46.576 ATOM 65.691 41.882 ATOM 235 CA LYS A 844 66.176 40.501 ATOM 236 C LYS A 844 67.635 40.390 1.854 1.00 77.20 ATOM 237 O LYS A 844 68.499 41.059 1.313 1.00 77.20 66.063 39.973 -0.045 1.00 63.87 ATOM 238 CB LYS A 844 67.921 39.570 ATOM 240 N LYS A 845 2.859 1.00 93.93 ATOM 241 CA LYS A 845 69.313 39.419 3.302 1.00 93.93 ATOM 242 C LYS A 845 69.979 38.431 2.382 1.00 93.93 ATOM 243 O LYS A 845 69.341 37.931 1.453 1.00 93.93 244 CB LYS A 845 69.391 38.854 4.684 1.00 20.96 ATOM ATOM 246 N ASP A 846 71.258 38.140 2.631 1.00 72.18 1.815 1.00 72.18 247 CA ASP A 846 71.912 37.136 ATOM 248 C 70.882 36.018 ATOM ASP A 846 2.059 1.00 72.18 249 0 70.861 35.389 3.129 1.00 72.18 ATOM ASP A 846 249 U ASP A 846 250 CB ASP A 846 251 CG ASP A 846 252 OD1 ASP A 846 253 OD2 ASP A 846 255 N GLY A 847 73.294 36.787 2.390 1.00100.00 ATOM 74.415 37.685 74.632 37.694 MOTA 1.842 1.00100.00 74.632 37.694 75.083 38.376 0.607 1.00100.00 ATOM ATOM 2.650 1.00100.00 69.992 35.836 1.082 1.00 99.53 ATOM MOTA 256 CA GLY A 847 68.923 34.870 1.231 1.00 99.53 ATOM 257 C GLY A 847 68.008 35.367 2.347 1.00 99.53 68.509 35.974 3.302 1.00 99.53 MOTA 258 O GLY A 847 MOTA 260 N LEU A 848 66.694 35.120 2.228 1.00 93.78 261 CA LEU A 848 65.670 35.542 3.212 1.00 93.78 ATOM 262 C LEU A 848 65.095 36.935 2.949 1.00 93.78 ATOM ATOM 263 O LEU A 848 65.825 37.878 2.662 1.00 93.78 ATOM 264 CB LEU A 848 66.215 35.504 4.654 1.00100.00 ATOM 265 CG LEU A 848 66.931 36.752 5.223 1.00100.00 266 CD1 LEU A 848 65.937 37.849 5.552 1.00100.00 ATOM ATOM 267 CD2 LEU A 848 67.719 36.377 6.472 1.00100.00 ATOM 269 N ARG A 849 63.781 37.063 3.070 1.00 80.14 ATOM 270 CA ARG A 849 63.127 38.347 2.855 1.00 80.14 271 C ARG A 849 62.191 38.669 4.013 1.00 80.14 MOTA MOTA 272 O ARG A 849 61.629 37.748 4.612 1.00 80.14

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ATOM	273	CB	ARG	ž.	849	62.320	38.327	1.561	1.00 99.23
ATOM	274	CG	ARG		849	61.390	37.148	1.452	1.00 99.23
ATOM	275	CD	ARG		849	60.021	37.392	2.081	1.00 99.23
	276	NE	ARG			59.022	36.466	1.540	1.00 99.23
MOTA					849	58.743	35.268	2.050	1.00 99.23
ATOM	277	CZ	ARG					3.127	1.00 99.23
ATOM	278		ARG		849	59.379	34.826		
ATOM	279	NH2			849	57.830	34.504	1.475	1.00 99.23
MOTA	286	N			850	62.041	39.958	4.350	1.00 26.65
ATOM	287	CA			850	61.122	40.332	5.425	1.00 26.65
ATOM	288	С			850	60.680	41.820	5.406	1.00 26.65
ATOM	289	0	MET	Α	850	60.502	42.468	4.345	1.00 26.65
ATOM	290	CB	MET	Α	850	61.743	39.999	6.780	1.00 99.56
ATOM	291	CG	MET	Α	850	63.156	39.475	6.689	1.00 99.56
ATOM	292	SD	MET	Α	850	64.190	40.566	5.745	1.00 99.56
ATOM	293	CE	MET	Α	850	65.522	40.771	6.902	1.00 99.56
ATOM	295	N	ASP	Α	851	60.515	42.341	6.612	1.00 27.82
MOTA	296	CA	ASP	Α	851	60.156	43.721	6.812	1.00 27.82
ATOM	297	C	ASP	Α	851	61.331	44.534	7.280	1.00 27.82
ATOM	298	ō			851	62.056	44.144	8.255	1.00 27.82
ATOM	299	CB			851	59.124	43.799	7.903	1.00 16.75
ATOM	300	CG	ASP		851	58.382	42.570	7.998	1.00 16.75
ATOM	301				851	58.147	42.049	6.837	1.00 16.75
ATOM	302	OD2	ASP		851	58.079	42.189	9.190	1.00 16.75
ATOM	304	N	ALA		852	61.420	45.691	6.635	1.00 37.08
ATOM	305	CA	ALA		852	62.400	46.719	6.887	1.00 37.08
			ALA				48.050	6.795	1.00 37.08
ATOM	306	C				61.643			1.00 37.08
ATOM	307	0	ALA			60.764	48.247	5.950	1.00100.00
ATOM	308	CB	ALA			63.471	46.663	5.835	
ATOM	310	N	ALA			61.955	48.986	7.663	1.00 97.32
ATOM	311	CA	ALA			61.303	50.269	7.528	1.00 97.32
ATOM	312	C	ALA			62.427	51.046	6.852	1.00 97.32
ATOM	313	0	ALA			63.501	51.201	7.415	1.00 97.32
ATOM	314	CB	ALA			60.947	50.824	8.895	1.00 15.46
ATOM	316	N	ILE	Α	854	62.187	51.469	5.617	1.00 84.85
ATOM	317	CA	ILE			63.178	52.179	4.810	1.00 84.85
ATOM	318	C	ILE	Α	854	63.221	53.682	4.985	1.00 84.85
ATOM	319	0	ILE	Α	854	62.197	54.334	5.006	1.00 84.85
ATOM	320	CB	ILE	Α	854	62.961	51.895	3.315	1.00 99.86
ATOM	321	CG1	ILE	A	854	63.540	50.538	2.948	1.00 99.86
ATOM	322	CG2	ILE	A	854	63.622	52.963	2.474	1.00 99.86
ATOM	323	CD1	ILE	Α	854	63.707	49.610	4.109	1.00 99.86
ATOM	325	N	LYS	A	855	64.426	54.228	5.095	1.00100.00
ATOM	326	CA	LYS	Α	855	64.602	55.666	5.249	1.00100.00
ATOM	327	C	LYS			65.867	56.179	4.602	1.00100.00
ATOM	328	0	LYS			66.915	55.567	4.710	1.00100.00
ATOM	329	CB			855	64.640	56.058	6.721	1.00100.00
ATOM	330	CG			855	65.352	57.373	6.977	1.00100.00
ATOM	331	CD	LYS			64.912	57.985	8.283	1.00100.00
ATOM	332	CE	LYS			65.371	57.143	9.459	1.00100.00
ATOM		NZ	LYS			66.801	57.366	9.812	1.00100.00
	333						57.314	3.927	1.00100.00
ATOM	338	N	ARG			65.751			
ATOM	339	CA	ARG			66.881	57.980	3.282	1.00100.00
ATOM	340	C	ARG			66.403	59.192	2.543	1.00100.00
ATOM	341	0	ARG			65.575	59.088	1.631	1.00100.00
ATOM	342	CB	ARG			67.602	57.089	2.279	1.00100.00
ATOM	343	CG	ARG			68.637	57.868	1.462	1.00100.00
ATOM	344	CD	ARG	A	856	68.118	58.410	0.090	1.00100.00

ATOM	345	NE	ARG A	056	68.946	59.472	-0.512	1.00100.00
ATOM	346	CZ	ARG A		68.938	59.819	-1.801	1.00100.00
ATOM	347		ARG A		68.145	59.210	-2.674	1.00100.00
ATOM	348	NH2			69.744	60.783	-2.222	1.00100.00
ATOM	355	Ñ	MET A		66.951	60.337	2.922	1.00100.00
ATOM	356	CA		857	66.567	61.616	2.275	1.00 39.23
ATOM	357	C	MET A		67.634	62.754	2.130	1.00 39.23
ATOM	358	ō		857	68.221	63.225	3.157	1.00 39.23
ATOM	359	CB	MET A		65.320	62.179	2.983	1.00100.00
ATOM	360	CG	MET A		64.305	62.877	2.092	1.00100.00
ATOM	361	SD	MET A		63.851	64.409	2.908	1.00100.00
ATOM	362	CE	MET A		61.992	64.355	2.935	1.00100.00
ATOM	363		MET A	857	67.842	63.172	0.963	1.00100.00
ATOM	365	N	ASP A	864	73.761	67.110	-3.548	1.00 99.95
ATOM	366	CA	ASP A		74.976	66.819	-4.350	1.00 99.95
ATOM	367	C	ASP A	864	76.224	67.493	-3.781	1.00 99.95
ATOM	368	0	ASP A	864	77.068	68.001	-4.530	1.00 99.95
ATOM	369	CB	ASP A	864	74.765	67.261	-5.839	1.00 2.00
ATOM	373	N	ASP A	865	76.338	67.492	-2.453	1.00100.00
ATOM	374	CA	ASP A	865	77.486	68.080	-1.760	1.00100.00
ATOM	375	C	ASP A	865	77.219	68.112	-0.267	1.00100.00
ATOM	376	0	ASP A	865	77.444	69.131	0.391	1.00100.00
ATOM	377	CB	ASP A	865	77.720	69.454	-2.255	1.00 53.42
ATOM	379	N	HIS A	866	76.752	66.983	0.263	1.00100.00
ATOM	380	CA	HIS A	866	76.397	66.853	1.678	1.00100.00
ATOM	381	C	HIS A	866	76.696	65.441	2.178	1.00100.00
ATOM	382	0	HIS A	866	75.859	64.777	2.805	1.00100.00
ATOM	383	CB	HIS A	866	74.905	67.144	1.848	1.00100.00
MOTA	384	CG	HIS A	866	74.036	66.378	0.896	1.00100.00
ATOM	385		HIS A		73.693	66.857	-0.350	1.00100.00
ATOM	386	CD2	HIS A	866	73.459	65.158	1.003	1.00100.00
ATOM	387		HIS A	866	72.943	65.965	-0.970	1.00100.00
ATOM	388		HIS A	866	72.787	64.925	-0.170	1.00100.00
ATOM	392	N	ARG A		77.912	64.998	1.913	1.00100.00
ATOM	393	CA	ARG A		78.335	63.673	2.300	1.00100.00
ATOM	394	C	ARG A		78.856	63.654	3.738	1.00100.00
ATOM	395	0	ARG A		80.061	63.597	3.985	1.00100.00
ATOM	396	CB	ARG A		79.393	63.206	1.310	1.00 99.71
ATOM	397	CG	ARG A		79.185	63.783	-0.098	1.00 99.71
ATOM	398	CD	ARG A	867	79.695	65.213	-0.213	1.00 99.71
ATOM	399	NE	ARG A		81.116	65.305	0.115	1.00 99.71
ATOM ATOM	400	CZ	ARG A	867	81.604	65.381	1.351	1.00 99.71
ATOM	401	NH1	ARG A	867	80.785	65.378	2.396	1.00 99.71
ATOM	409	NH2 N		867	82.919	65.450	1.540	1.00 99.71
ATOM	410	CA	ASP A	868 868	77.920 78.239	63.713 63.706	4.683	1.00 88.85
ATOM	411	CM	ASP A	868	77.969		6.112	
ATOM	412	0	ASP A	868	78.558	62.278 61.850	6.646 7.655	1.00 88.85
ATOM	413	CB	ASP A	868	77.368	64.758		
	414	CG	ASP A	868	77.674	66.231	6.870 6.460	1.00 67.57
ATOM	415		ASP A	868	78.671	66.496	5.753	1.00 67.57
ATOM	416	OD2	ASP A	868	76.914	67.142	6.852	1.00 67.57
ATOM	418	N	PHE A	869	77.097	61.545	5.943	1.00100.00
ATOM	419	CA	PHE A	869	76.719	60.176	6.322	1.00100.00
ATOM	420	C	PHE A	869	77.809	59.128	6.086	1.00100.00
ATOM	421	0	PHE A	869	78.433	59.091	5.017	1.00100.00
ATOM	422	CB	PHE A	869	75.431	59.745	5.595	1.00100.00
						,,,,,	2.223	2.00 20.24

ATOM	423	CG	PHE A	869	75.346	60.207	4.164	1.00 98.24
ATOM	424	CD1	PHE A	869	74.434	61.186	3.789	1.00 98.24
ATOM	425	CD2	PHE A		76.165	59.652	3.186	1.00 98.24
ATOM	426	CEl	PHE A		74.341	61.604	2.457	1.00 98.24
ATOM	427	CE2	PHE A		76.078	60.063	1.854	1.00 98.24
MOTA	428	CZ	PHE A		75.166	61.038	1.492	1.00 98.24
MOTA	430	N	ALA A		78.007	58.287	7.106	1.00100.00
ATOM	431	CA	ALA A		79.005	57.205	7.146	1.00100.00
MCTA	432	C	ALA A		79.570	57.201	8.564	1.00100.00
ATOM	433	0	ALA A	870	80.736	56.892	8.807	1.00100.00
ATOM	434	CB	ALA A	870	80.131	57.437	6.134	1.00100.00
MCTA	436	N	GLY A	871	78.706	57.575	9.490	1.00100.00
ATOM	437	CA	GLY A	871	79.058	57.626	10.888	1.00100.00
ATOM	438	C	GLY A	871	77.783	57.234	11.591	1.00100.00
ATOM	439	0	GLY A		77.802	56.636	12.662	1.00100.00
ATOM	441	N	GLU A		76.656	57.592	10.987	1.00100.00
MOTA	442	CA	GLU A		75.384	57.210	11.564	1.00100.00
ATOM	443	C	GLU A		75.581	55.695	11.584	1.00100.00
ATOM	444	ō	GLU 2		75.628	55.083	12.655	1.00100.00
ATOM	445	CB	GLU A	872	74.200	57.613	10.651	1.00 99.93
ATOM	446	CG	GLU A		73.244	58.668	11.260	1.00 99.93
ATOM	447	CD	GLU A		71.754	58.458	10.919	1.00 99.93
ATOM	448	OE1	GLU A		71.434	57.633	10.040	1.00 99.93
ATOM	449	OE2	GLU A		70.894	59.128	11.532	1.00 99.93
ATÓM	451	N	LEU A		75.773	55.121	10.389	1.00 77.06
ATOM	452	CA	LEU F		75.982	53.683	10.215	1.00 77.06
ATOM	453	C	LEU A		77.167	53.198	11.046	1.00 77.06
ATOM	454	Ö	LEU A		77.384	51.998	11.180	1.00 77.06
ATOM	455	CB	LEU A	873	76.202	53.366	8.746	1.00 96.97
ATOM	457	Ñ	GLU 2		77.920	54.142	11.612	1.00 98.87
ATOM	458	CA	GLU A	874	79.091	53.832	12.423	1.00 98.87
ATOM	459	C	GLU A	874	78.740	53.585	13.890	1.00 98.87
ATOM	460	0	GLU A	874	79.072	52.546	14.449	1.00 98.87
ATOM	461	CB	GLU A	874	80.107	54.954	12.306	1.00 56.03
ATOM	463	N	VAL A	875	78.096	54.541	14.543	1.00100.00
ATOM	464	CA	VAL A	875	77.725	54.320	15.936	1.00100.00
ATOM	465	С	VAL A	875	76.577	53.312	15.875	1.00100.00
ATOM	466	0	VAL A	875	76.533	52.370	16.654	1.00100.00
ATOM	467	CB	VAL A	875	77.279	55.629	16.582	1.00100.00
ATOM	469	N	LEU A	876	75.678	53.520	14.911	1.00 63.64
MOTA	470	CA	LEU A	876	74.515	52.662	14.649	1.00 63.64
ATOM	471	C	LEU A	876	74.825	51.155	14.638	1.00 63.64
ATOM	472	0	LEU A		73.935	50.359	14.292	1.00 63.64
ATOM	473	CB	LEU A	876	73.914	53.005	13.267	1.00 36.83
ATOM	474	CG	LEU A	876	72.851	54.076	12.997	1.00 36.83
ATOM	475	CD1	LEU A	876	72.028	53.665	11.807	1.00 36.83
ATOM	476	CD2	LEU A	876	71.987	54.260	14.181	1.00 36.83
ATOM	478	N	CYS A	877	76.072	50.786	14.978	1.00 75.85
ATOM	479	CA	CYS F	877	76.570	49.391	14.973	1.00 75.85
ATOM	480	C	CYS A	877	76.791	48.697	16.317	1.00 75.85
MOTA	481	0	CYS A	877	75.965	47.904	16.771	1.00 75.85
ATOM	482	CB	CYS A	877	77.890	49.343	14.202	1.00 82.25
MCTA	483	SG	CYS A	877	78.205	50.859	13.250	1.00 82.25
MOTA	485	N	LYS A	878	77.947	48.968	16.913	1.00100.00
ATOM	486	CA	LYS A	878	78.334	48.400	18.202	1.00100.00
MOTA	487	C	LYS A	878	77.159	48.295	19.186	1.00100.00
MOTA	488	0	LYS A	878	77.237	47.565	20.178	1.00100.00

Docket/App No.: 2079.1037-001

Title: Method of Identifying Inhibitors of TIE-2 Inventors: Nancy J. Bump *et al.*

489 CB LYS A 878 MOTA 79.460 49.251 18.826 1.00 99.60 80.588 49.643 17.842 1.00 99.60 ATOM 490 CG LYS A 878 MOTA 491 CD LYS A 878 80.814 51.160 17.739 1.00 99.60 MOTA 492 CE LYS A 878 81.033 51.598 16.292 1.00 99.60 ATOM 493 NZ LYS A 878 82.152 52.567 16.077 1.00 99.60 498 N ATOM LEU A 879 76.079 49.024 18.905 1.00 99.14 499 CA LEU A 879 ATOM 74.905 49.034 19.762 3.00 99.14 ATOM 500 C LEU A 879 73.664 48.687 18.953 1.00 99.14 ATOM 501 0 72.574 48.526 19.488 1.00 99.14 LEU A 879 ATOM 502 CB LEU A 879 74.748 50.416 20.401 1.00 99.96 ATOM 503 CG LEU A 879 74.125 51.546 1.00 99.96 19.579 MOTA 504 CD1 LEU A 879 74.530 52.863 20.154 1.00 99.96 ATOM 505 CD2 LEU A 879 74.555 51.454 1.00 99.96 18.135 ATOM 507 N GLY A 880 73.840 48.593 1.00 74.75 17.647 ATOM 508 CA GLY A 880 72.737 48.256 16.775 1.00 74.75 ATOM 509 C GLY A 880 71.778 47.281 17.406 1.00 74.75 ATOM 510 0 GLY A 880 70.589 47.458 17.285 1.00 74.75 512 N ATOM HIS A 881 72.288 46.243 18.067 1.00100.00 ATOM 513 CA HIS A 881 514 C HIS A 881 71.428 45.246 18.700 1.00100.00 ATOM 71.274 45.583 20.172 1.00100.00 ATOM 515 0 HIS A 881 71.798 46.571 20.661 1.00100.00 516 CB HIS A 881 ATOM 71.989 43.818 18.514 1.00 80.74 517 CG 41S A 881 ATOM 71.360 42.778 19.401 1.00 80.74 ATOM 518 ND1 HIS A 881 70.116 42.234 19.155 1.00 80.74 ATOM 519 CD2 HIS A 881 71.778 42.230 20.573 1.00 80.74 ATOM 520 CE1 HIS A 881 69.792 41.404 20.133 1.00 80.74 521 NE2 HIS A 881 ATOM 70.783 41.384 21.007 1.00 80.74 ATOM 525 N HIS A 882 70.539 44.718 20.846 1.00 5.03 ATOM 526 CA HIS A 882 70.126 44.779 22.266 1.00 5.03 ATOM 527 C HIS A 882 68.572 44.646 22.018 1.00 5.03 ATOM 528 O HIS A 882 67.998 45.211 20.996 1.00 5.03 ATOM 529 CB HIS A 882 70.487 46.161 22.887 1.00 36.20 ATOM 530 CG HIS A 882 70.085 46.316 24.322 1.00 36.20 ATOM 531 ND1 HIS A 882 68.786 46.169 24.753 1.00 36.20 ATOM 532 CD2 HIS A 882 70.816 46.553 25.432 1.00 36.20 533 CE1 HIS A 882 ATOM 68.731 46.302 26.066 1.00 36.20 ATOM 534 NE2 HIS A 882 69.949 46.535 26.504 1.00 36.20 ATOM 538 N PRO A 883 67.875 43.928 22.885 1.00 18.79 ATOM 539 CA PRO A 883 66.444 43.868 22.564 1.00 18.79 ATOM 540 C PRO A 883 65.806 45.252 22.201 1.00 18.79 PRO A 883 ATOM 541 0 65.014 45.404 21.188 1.00 18.79 ATOM 542 CB PRO A 883 65.804 43.294 23.829 1.00 41.14 ATOM 543 CG PRO A 883 66.946 43.069 24.810 1.00 41.14 ATOM 544 CD PRO A 883 68.231 43.209 24.107 1.00 41.14 ATOM 545 N ASN A 884 66.245 46.252 22.975 1.00 21.27 546 CA ASN A 884 ATOM 65.656 47.545 22.910 1.00 21.27 ATOM 547 C ASN A 884 66.055 48.782 22.174 1.00 21.27 ATOM 548 0 ASN A 884 65.930 49.811 22.738 1.00 21.27 ATOM 549 CB ASN A 884 65.371 47.916 24.332 1.00 47.99 ATOM 550 CG ASN A 884 64.926 46.747 25.093 1.00 47.99 ATOM 551 OD1 ASN A 884 65.360 46.508 26.173 1.00 47.99 ATOM 552 ND2 ASN A 884 1.00 47.99 64.056 45.990 24.504 ATOM 556 N ILE A 885 66.421 48.685 20.906 1.00 2.00 CA ILE A 885 ATOM 557 66.784 49.799 20.139 1.00 2.00 MOTA 558 C ILE A 885 66.578 49.337 18.712 1.00 2.00 ATOM 559 0 ILE A 885 67.324 48.601 18.278 1.00 2.00 ATOM 560 CB ILE A 885 68.282 50.142 20.404 1.00 5.30

ATOM	561	CG1	ILE /	Ď,	885	68.387	50.790	21.774	1.00 5.30
ATOM	562	CG2	ILE 2	Ą	885	68.946	51.096	19.301	1.00 5.30
ATOM	563	CD1	ILE A	Ą	885	69.834	51.062	22.137	1.00 5.30
ATOM	565	N	ILE A	Ą.	886	65.634	49.811	17.931	1.00 41.79
ATOM	566	CA	ILE A	ą.	886	65.528	49.296	16.564	1.00 41.79
ATOM	567	С	ILE A	Ą	886	66.883	48.887	15.937	1.00 41.79
ATOM	568	0	ILE A	ą.	886	67.899	49.217	16.450	1.00 41.79
ATOM	569	CB	ILE A	Z,	886	64.769	50.316	15.671	1.00 97.62
ATOM	570	CG1	ILE A	Ą	886	63.737	49.563	14.817	1.00 97.62
ATOM	571	CG2	ILE A	A	886	65.742	51.141	14.871	1.00 97.62
ATOM	572	CD1	ILE A	Ą	886	62.833	50.438	14.004	1.00 97.62
ATOM	574	N	ASN A	Ą	887	66.915	48.190	14.817	1.00 58.02
ATOM	575	CA	ASN A	A.	887	68.191	47.751	14.300	1.00 58.02
ATOM	576	C	ASN 3	A.	887	68.481	48.230	12.940	1.00 58.02
ATOM	577	0	ASN A	A	887	67.635	48.811	12.321	1.00 58.02
ATOM	578	CB	ASN A			68.237	46.228	14.269	1.00 61.11
ATOM	579	CG	ASN A			69.626	45.688	14.460	1.00 61.11
ATOM	580	OD1	ASN A	A	887	70.307	45.367	13.505	1.00 61.11
ATOM	581	ND2	ASN A			70.050	45.584	15.711	1.00 61.11
ATOM	585	N	LEU 2			69.688	47.945	12.467	1.00100.00
ATOM	586	CA	LEU A			70.097	48.313	11.122	1.00100.00
ATOM	587	c.	LEU			70.158	47.037	10.282	1.00100.00
ATOM	588	0	LEU			71.039	46.202	10.444	1.00100.00
ATOM	589	CB	LEU :		888	71.467	48.993	11.131	1.00100.00
ATOM	590	CG	LEU .			72.068	49.217	9.743	1.00100.00
ATOM	591		LEU		888	72.054	50.676	9.410	1.00100.00
ATOM	592		LEU .			73.475	48.686	9.699	1.00100.00
MCTA	594	N	LEU .			69.191	46.880	9.398	1.00 73.18
ATOM	595	CA	LEU .		889	69.128	45.721	8.530	1.00 73.18
ATOM	596	C	LEU .		889	70.044	45.860	7.290	1.00 73.18
ATOM	597	0	LEU .		889	70.737	44.920	6.926	1.00 73.18
ATOM	598	CB	LEU .			67.666	45.500	8.102	1.00 10.03
ATOM	599	CG	LEU .		889	66.628	44.729	9.010	1.00 10.03
ATOM	600	CD1	LEU .		889	66.180	43.517	8.146	1.00 10.03
ATOM	601		LEU .			67.147	44.336	10.432	1.00 10.03
ATOM	603	N N	GLY .		890	70.058	47.028	6.651	1.00100.00
ATOM	604	CA	GLY .			70.898	47.201	5.475	1.00100.00
ATOM	605	C	GLY .			71.057	48.582	4.845	1.00100.00
ATOM	606	0	GLY			70.515	49.581	5.319	1.00100.00
ATOM	608	N	ALA			71.829	48.616	3.758	1.00 93.61
ATOM	609	CA	ALA			72.124	49.833	2.992	1.00 93.61
ATOM	610	CA	ALA			73.124	49.438	1.929	1.00 93.61
			ALA			73.123	48.626	2.223	1.00 93.61
ATOM	611	0	ALA			72.763	50.871	3.886	1.00 28.61
ATOM	612	CB	CYS			73.033	49.985	0.715	1.00100.00
ATOM	614	N				74.034	49.965	-0.306	1.00100.00
ATOM	615	CA	CYS						1.00100.00
ATOM	616	С	CYS			74.789	50.793	-0.956	1.00100.00
MCTA	617	0	CYS			75.934	51.073	-0.606	1.00100.00
ATOM	618	CB	CYS			73.432	48.787	-1.429	1.00100.00
ATOM	619	SG	CYS			74.641	48.356	-2.757	
ATOM	621	74	GLU			74.134	51.447	-1.914	1.00 85.23
ATOM	622	CA	GLU			74.715	52.555	-2.679	1.00 85.23
ATOM	623	C	GLU			73.816	52.794	-3.880	1.00 85.23
ATOM	624	0	GLU			74.228	52.512	-5.011	
ATOM	625	CB	GLU			76.108	52.176	-3.222	1.00100.00
ATOM	626	CG	GLU			77.267	53.065	-2.785	1.00100.00
ATOM	627	CD	GLU	А	893	78.487	52.246	-2.386	1.00100.00

ATOM	628	OE1	GLU	Α	893	79.029	51.535	-3.266	1.00100.00
ATOM	629	OE2	GLU	Α	893	78.893	52.307	-1.197	1.00100.00
ATOM	631	K	HIS	Α	894	72.602	53.293	-3.664	1.00100.00
ATOM	632	CA	HIS			71.731	53.508	-4.810	1.00100.00
ATOM	633	C	HIS		894	71.885	54.855	-5.463	1.00100.00
MOTA	634	ō	HIS			71.106	55.770	-5.181	1.00100.00
ATOM	635	CB	HIS			70.261	53.338	-4.477	1.00100.00
ATOM	636	CG	HIS						
ATOM	637					69.370	53.597	-5.652	1.00100.00
			HIS			68.309	54.476	-5.610	1.00100.00
ATOM	638		HIS			69.419	53.128	-6.922	1.00100.00
MOTA	639		HIS			67.743	54.539	-6.802	1.00100.00
ATOM	640		HIS			68.397	53.729	-7.615	1.00100.00
ATOM	644	N	ARG			72.888	54.950	-6.340	1.00100.00
ATOM	€45	CA	ARG			73.176	56.161	-7.090	1.00100.00
MOTA	646	C	ARG			72.331	57.309	-6.481	1.00100.00
MOTA	647	0	ARG	Α	895	71.194	57.562	-6.910	1.00100.00
ATOM	648	CB	ARG	Α	895	72.842	55.883	-8.571	1.00 36.65
ATOM	649	CG	ARG	A.	895	73.711	54.767	-9.229	1.00 36.65
MOTA	650	CD	ARG	Α	895	73.012	54.079	-10.421	1.00 36.65
ATOM	651	NE	ARG	Α	895	73.587		-11.738	1.00 36.65
ATOM	652	CZ	ARG	Д	895	74.382		-12.451	1.00 36.65
ATOM	653	NH1	ARG			74.735	52.315	-11.986	1.00 36.65
ATOM	654	NH2	ARG			74.848		-13.644	1.00 36.65
ATOM	661	N	GLY			72.901	57.979	-5.469	1.00 33.20
ATOM	662	CA	GLY			72.190	59.016	-4.751	1.00 33.20
ATOM	663	C	GLY			71.918	58.455	-3.348	1.00 33.20
ATOM	664	0	GLY			70.779	58.462	-2.847	
ATOM	666	N	TYR			72.971	57.947		
ATOM	667	CA	TYR			72.864		-2.705	1.00 98.45
ATOM	668	CA	TYR				57.372	-1.356	1.00 98.45
ATOM	669	0				72.959	55.835	-1.387	1.00 98.45
ATOM	670	CB	TYR			73.599	55.240	-2.258	1.00 98.45
ATOM			TYR			71.532	57.786	-0.716	1.00100.00
	671	CG	TYR			71.522	58.208	0.734	1.00100.00
ATOM	672	CD1	TYR			71.152	59.511	1.080	1.00100.00
MOTA	673	CD2	TYR			71.631	57.268	1.756	1.00100.00
MOTA	674	CE1	TYR			70.860	59.866	2.391	1.00100.00
ATOM	675	CE2	TYR			71.345	57.604	3.074	1.00100.00
MOTA	676	CZ	TYR			70.947	58.908	3.389	1.00100.00
MOTA	677	OH	TYR			70.582	59.246	4.682	1.00100.00
MOTA	680	N	LEU	Α	898.	72.293	55.212	-0.419	1.00100.00
ATOM	681	CA	LEU	A	898	72.272	53.765	-0.258	1.00100.00
ATOM	682	C	LEU	A	898	70.983	53.363	0.469	1.00100.00
ATOM	683	0	LEU	Α	898	70.810	52.197	0.836	1.00100.00
ATOM	684	CB	LEU	Α	898	73.495	53.328	0.551	1.00 67.92
ATOM	686	N	TYR	A	899	70.097	54.345	0.668	1.00100.00
ATOM	687	CA	TYR			68.813	54.169	1.347	1.00100.00
ATOM	688	С	TYR			68,976	53.434	2.680	1.00100.00
ATOM	689	ō	TYR			70.090	53.252	3.153	1.00100.00
ATOM	690	CB	TYR			67.840	53.420	0.434	1.00 99.94
ATOM	691	CG	TYR			67.265	54.259	-0.694	1.00 99.94
ATOM	692	CD1	TYR			67.218	53.770	-2.004	1.00 99.94
ATOM	693	CD2	TYR			66.738	55.531	-0.454	1.00 99.94
ATOM	694	CE1	TYR			66.662	54.519	~3.044	1.00 99.94
ATOM	695	CE2	TYR			66.176	56.295	-1.493	1.00 99.94
ATOM	696	CZ	TYR			66.143	55.778		1.00 99.94
ATOM	697	OH	TYR			65.580	56.509	-2.780 -3.792	1.00 99.94
ATOM	700	N	LEU			67.876	53.017	3.300	1.00 99.94
		-1	-120	~	200	07.076	JJ. UI/	2.300	1.00 33.32

ATOM	701								
		CA C	LEU			67.987	52.305	4.573	1.00 99.32
ATOM	702		LEU			67.119	51.071	4.770	1.00 99.32
ATOM	703	0	LEU		900	66.306	50.702	3.933	1.00 99.32
MOTA	704	CB	LEU			67.755	53.258	5.752	1.00 72.65
ATOM	705	CG	LEU			68.911	53.350	6.752	1.00 72.65
ATOM	706				900	70.175	52.843	6.059	1.00 72.65
ATOM	707		LEU .		900	69.096	54.792	7.259	1.00 72.65
ATOM	709	7.1	ALA .		901	67.330	50.439	5.912	1.00100.00
ATOM	710	CA	ALA.			66.617	49.244	6.288	1.00100.00
ATOM	711	C	ALA .			66.802	49.053	7.774	1.00100.00
ATOM	712	0	ALA .	Α	901	67.774	48.484	8.231	1.00100.00
ATOM	713	CB	ALA .	Α	901	67.152	48.049	5.537	1.00100.00
ATOM	715	N	ILE .	Α	902	65.840	49.575	8.510	1.00 33.23
ATOM	716	CA	ILE .	Α	902	65.773	49.510	9.964	1.00 33.23
ATOM	717	C	ILE .	Α	902	64.912	48.295	10.352	1.00 33.23
ATOM	718	0	ILE .	Α	902	63.988	47.959	9.648	1.00 33.23
MOTA	719	CB	ILE .	Α	902	65.130	50.817	10.474	1.00 58.03
ATOM	720	CG1	ILE .	A	902	65.930	51.992	9.960	1.00 58.03
ATOM	721	CG2	ILE .			65.107	50.870	11.955	1.00 58.03
ATOM	722	CD1	ILE .			67.193	52.207	10.738	1.00 58.03
ATOM	724	N	GLU .			65.256	47.622	11.440	1.00 37.33
ATOM	725	CA	GLU :			64.468	46.507	11.912	1.00 37.33
ATOM	726	C	GLU			63.079	47.051	11.790	1.00 37.33
ATOM	727	ō	GLU ,			62.856	48.198	12.081	1.00 37.33
ATOM	728	CB	GLU .						
ATOM	729	CG				64.732	46.216	13.388	1.00 74.67
ATOM	730	CD	GLU A		903	63.667	45.362	14.022	1.00 74.67
ATOM	731	OE1				63.757	45.302	15.525	1.00 74.67
ATOM						62.771	44.921	16.178	1.00 74.67
	732		GLU .			64.809	45.637	16.072	1.00 74.67
ATOM	734	N	TYR :			62.137	46.221	11.362	1.00 98.95
ATOM	735	CA	TYR .			60.765	46.667	11.209	1.00 98.95
ATOM	736	C	TYR I			59.912	46.319	12.435	1.00 98.95
ATOM	737	0	TYR I			59.998	45.210	12.968	1.00 98.95
ATOM	738	CB	TYR ;			60.187	46.064	9.939	1.00 65.21
MOTA	739	CG	TYR 3			58.741	46.366	9.749	1.00 65.21
ATOM	740	CD1	TYR :			58.343	47.461	9.002	1.00 65.21
ATOM	741	CD2	TYR A	Ą.	904	57.760	45.602	10.367	1.00 65.21
ATOM	742	CEl	TYR :	Ą	904	56.994	47.797	8.878	1.00 65.21
ATOM	743	CE2	TYR A			56.418	45.929	10.249	1.00 65.21
ATOM	744	CZ	TYR I	Ą	904	56.046	47.029	9.500	1.00 65.21
ATOM	745	OH	TYR 2	Ď,	904	54.736	47.335	9.321	1.00 65.21
ATOM	748	И	ALA 3	Ą	905	59.103	47.287	12.877	1.00 44.07
ATOM	749	CA	ALA i	D,	905	58.241	47.148	14.049	1.00 44.07
ATOM	750	C	ALA I	A	905	56.742	46.973	13.670	1.00 44.07
ATOM	751	0	ALA I	Ą	905	56.091	47.865	13.125	1.00 44.07
ATOM	752	CB	ALA :			58.459	48.326	14.943	1.00 44.16
ATOM	754	N	PRO A	Ą	906	56.169	45.798	13.983	1.00 95.76
ATOM	755	CA	PRO I	D.	906	54.773	45.513	13.643	1.00 95.76
ATOM	756	C	PRO I		906	53.627	46.336	14.226	1.00 95.76
ATOM	757	ō	PRO I		906	52.547	46.358	13.656	1.00 95.76
ATOM	758	CB	PRO I		906	54.642	44.022	13.056	1.00 74.50
ATOM	759	CG	PRO I		906	55.605	43.816	15.072	1.00 74.50
ATOM	760	CD	PRO I		906	56.773	44.682	14.734	1.00 74.50
ATOM	761	N	HIS A			53.838	47.018		
ATOM	762	CA.	HIS A		907	52.751	47.018	15.336 15.909	1.00 75.88
ATOM	763	CA	HIS A			52.751			1.00 75.88
ATOM	764	0	HIS A			52.370	49.300	15.917	1.00 75.88
	/04	9	****** 1		201	24.370	49.979	16.754	1.00 75.88

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Title: Method of Identifying Inhibitors of TIE-2 Inventors: Nancy J. Bump *et al.*

ATOM	765	CB	HIS	Α	907	52.491	47.321	17.327	1.00	58.13
ATOM	766	CG	HIS			52.494	45.839	17.465		58.13
ATOM	767	ND1	HIS			52.400	44.991	16.387	1.00	58.13
ATOM	768		HIS		907	52.595	45.049	18.552		58.13
ATOM	769	CE1	Hls		907	52.442	43.741	16.805	1.00	
ATOM	770		HIS		907	52.563	43.750	18.117	1.00	58.13
ATOM	774	N	GLY			53.744	49.827	15.004	1.00	99.49
ATOM	775	CA	GLY			53.952	51.258	14.965	1.00	99.49
ATOM	776	C	GLY	Α	908	54.688	51.796	16.168	1.00	99.49
ATOM	777	0	GLY	Α	908	55.536	51.126	16.736	1.00	99.49
ATOM	779	N	ASN	Α	909	54.345	53.015	16.565	1.00	37.36
ATOM	780	CA	ASN	А	909	54.995	53.672	17.686	1.00	37.36
ATOM	781	C	ASN	А	909	54.274	53.675	18.970	1.00	37.36
ATOM	782	0	ASN	Α	909	53.091	53.524	19.093	1.00	37.36
ATOM	783	CB	ASN	Α	909	55.422	55.139	17.378	1.00	21.80
ATOM	784	CG	ASN	Α	909	54.300	56.174	17.594	1.00	21.80
ATOM	785	OD1	ASN	Α	909	54.091	57.036	16.763	1.00	21.80
ATOM	786	ND2	ASN	А	909	53.611	56.094	18.714	1.00	21.80
ATOM	790	N	LEU	Α	910	55.043	53.958	19.971	1.00	6.05
ATOM	791	CA	LEU	Α	910	54.505	53.895	21.258	1.00	6.05
ATOM	792	C	LEU	Α	910	53.372	54.836	21.506	1.00	6.05
ATOM	793	0	LEU	Α	910	52.558	54.488	22.290	1.00	6.05
ATOM	794	CB	LEU	Α	910	55.629	53.964	22.304	1.00	22.43
ATOM	795	CG	LEU	А	910	55.112	53.756	23.738	1.00	22.43
ATOM	796	CDI	LEU	А	910	54.795	52.285	23.989	1.00	22.43
ATOM	797	CD2	LEU	Α	910	56.128	54.383	24.829	1.00	22.43
ATOM	799	N	LEU	Α	911	53.269	56.034	20.959	1.00	53.76
ATOM	800	CA.	LEU	A	911	52.062	56.772	21.333	1.00	53.76
ATOM	801	C	LEU	Α	911	50.801	56.136	20.690	1.00	53.76
ATOM	802	0	LEU	Α	911	49.969	55.583	21.406	1.00	53.76
ATOM	803	CB	LEU	A	911	52.158	58.265	20.991	1.00	2.16
MOTA	804	CG	LEU		911	51.350	59.370	21.692	1.00	2.16
ATOM	805		PEA			51.622	59.513	23.075	1.00	2.16
ATOM	806	CD2				51.612	60.569	20.997	1.00	2.16
ATOM	808	N			912	50.666	56.165	19.363		37.67
ATOM	809	CA	ASP			49.481	55.594	18.764	1.00	37.67
ATOM	810	C	ASP			49.087	54.287	19.391	1.00	37.67
MOTA	811	0	ASP		912	48.010	54.116	19.875	1.00	37.67
ATOM	812	CB	ASP		912	49.652	55.383	17.285	1.00	2.00
ATOM	813	CG	ASP		912	49.965	56.675	16.516	1.00	2.00
ATOM	814		ASP		912	49.929	56.718	15.258	1.00	2.00
MOTA	815	OD2			912	50.263	57.647	17.195	1.00	2.00
ATOM	817	N	PHE			49.977	53.341	19.403		21.37
MOTA	818	CA			913	49.659	52.056	19.975	1.00	21.37
ATOM	819	C	PHE			49.216	52.291	21.331	1.00	21.37
ATOM	820	0	PHE			48.338	51.566	21.787		21.37
ATOM	821	CB			913	50.826	51.097	19.956	1.00	2.23
MOTA	822	CG			913	50.639	49.861	20.776	1.00	2.23
ATOM	823	CD1			913	50.389	48.681	20.185	1.00	2.23
ATOM	824	CD2			913	50.826	49.886	22.142	1.00	2.23
ATOM	825	CEI	PHE			50.330	47.610	20.870	1.00	2.23
ATOM	826	CE2			913	50.749	48.684	22.902	1.00	2.23
ATOM ATOM	827	CZ	PHE			50.503	47.593	22.238	1.00	2.23
	829	N	LEU	Æ,	コエゼ	49.753	53.295	22.003	1.00	34.44
			7 777~	2	0.1.4	40 222	ED FFO	22 242	2 0 0	24 44
ATOM	830	CA	LEU			49.233	53.552	23.340	1.00	34.44
			LEU	A	914	49.233 47.770 46.927	53.552 54.028 53.718	23.340 23.202 24.017	1.00	34.44 34.44 34.44

ATOM	833	CB	LEU	JΑ	914	50.0	189	54.600	24.053	1 00	99.33
ATOM	834	CG			914	51.		54.077	24.972		99.33
ATOM	835	CDI			914	52.3		55.032	24.979		99.33
ATOM	836	CD2			914	50.6		53.912	26.367		99.33
ATOM	838	N			915	47.4		54.720	22.111	1.00	
ATOM	839	CA			915	46.2		55.332	21.795		
ATOM	840	C			915	45.0		54.463	21.793	1.00	
ATOM	841	0			915	43.8		54.728	21.700		
ATOM	842	CB			915	46.4		56.347	20.720	1.00	
ATOM	843	CG			915	46.6		57.788		1.00	6.43
ATOM	844	CD			915	47.9		58.402	21.276	1.00	6.43
MOTA	845	NE			915	48.0		59.491	21.097	1.00	6.43
MOTA	846	CZ			915	48.2			22.107	1.00	6.43
ATOM	847		ARG			48.3		50.805 51.314	21.838	1.00	6.43
ATOM	848	NH2			915	48.4		51.514	20.610	1.00	6.43
ATOM	855	N	LYS		916	45.3			22.822	1.00	6.43
ATOM	856	CA	LYS			44.5		33.475	20.520		22.32
ATOM	857	C			916			52.462	20.007		22.32
ATOM	858	o	LYS		916	44.1		51.432	21.156		22.32
ATOM	859	CB			916	43.6		0.278	20.864		22.32
ATOM	860	CG			916	45.2		1.740	18.908		23.97
ATOM	861	CD			916	46.7		1.281	19.327		23.97
ATOM	862	CE			916	46.8		0.099	20.472		23.97
ATOM	863	NZ			916	46.8		8.726	19.880		23.97
ATOM	868	N				46.6		8.934	18.374		23.97
ATOM	869	CA			917	44.3		1.831	22.418		22.74
ATOM	870	C			917	44.1		1.001	23.600		22.74
ATOM	871				917	43.0		1.499	24.516		22.74
ATOM	872	O CB			917	42.6		0.829	25.545		22.74
ATOM					917	45.4		0.997	24.415		34.41
ATOM	873 876	OG			917	45.3		0.676	25.795		34.41
ATOM		N	ARG			42.6		2.718	24.199		59.16
	877	CA	ARG			41.5		3.402	24.928	1.00	59.16
ATOM	878	C	ARG			40.2		2.937	24.293		59.16
ATOM	879	0	ARG			39.6		3.636	23.457	1.00	59.16
ATOM	880	CB	ARG			41.7		4.919	24.780	1.00	47.25
ATOM	881	CG	ARG			43.1		5.447	25.013	1.00	47.25
ATOM	882	CD	ARG			43.2		6.981	25.073	1.00	47.25
ATOM	883	NE	ARG			44.0	53 5	7.501	26.186	1.00	47.25
MOTA	884	CZ	ARG			44.3		8.794	26.368	1.00	47.25
ATOM	885	NH1				43.8	94 5	9.671	25.521	1.00	47.25
ATOM	886	NH2	ARG		918	45.0		9.226	27.374	1.00	47.25
ATOM	893	N	VAL			39.82		1.722	24.665	1.00	99.87
ATOM	894	CA	VAL			38.62		1.077	24.148	1.00	99.87
MOTA	895	C	VAL			37.44	2 5	2.049	24.208		99.87
ATOM	896	0	VAL			36.84	9 5	2.376	23.191	1.00	99.87
ATOM	897	CB	VAL			38.31	75 4	9.713	24.883	1.00	30.60
ATOM	898		VAL			39.00	7 4	8.626	24.110	1.00	
ATOM	899		VAL			38.94	9 4	9.723	26.257	1.00	
ATOM	901	N	LEU	Α	920	37.13	.1 5	2.497	25.405	1.00	36.31
ATOM	902	CA	LEU			36.13		3.513	25.648		36.31
ATOM	903	C	LEU			36.53		4.698	24.811		36.31
MOTA	904	0	LEU	A	920	37.06		5.646	25.312		36.31
MOTA	905	CB	LEU	A	920	36.20		3.928	27.088		11.95
ATOM	906	CG	LEU	Α	920	34.95		4.248	27.902		11.95
ATOM	907	CD1	LEU	Α	920	34.64		2.948	28.585		11.95
ATOM	908		LEU			35.11		5.350	28.954		11.95
ATOM	910	N	GLU			36.34		4.626	23.518	1.00	

ATOM	911	CA	GLU A	921	36.726	55.656	22.606	1.00 9.77
ATOM	912	C	GLU /		36.937	54.877	21.314	1.00 9.77
ATOM	913	ō	GLU A		36.305	55.139	20.294	1.00 9.77
ATOM	914	CB	GLU A		38.009	56.321	23.076	1.00 41.44
ATOM	915	CG	GLU A		38.187	57.798	22.646	1.00 41.44
ATOM	916	CD	GLU A		39.514	58.054	21.899	1.00 41.44
ATOM	917	OE1	GLU A		40.583	58.228	22.581	1.00 41.44
ATOM	918	OE2	GLU A		39.465	58.066	20.642	1.00 41.44
ATOM	920	N	THR F		37.799	53.864	21.348	1.00 38.88
ATOM	921	CA	THR A		38.110	53.051	20.167	1.00 38.88
ATOM	922	C	THR A		36.981	52.136	19.842	1.00 38.88
ATOM	923	0	THR A		36.505	52.013	18.726	1.00 38.88
ATOM	924	СВ	THR A		39.174	52.111	20.500	1.00 40.90
ATOM	925	OG1	THR F		39.068	51.846	21.908	1.00 40.90
ATOM	926	CG2	THR A		40.560	52.671	20.140	1.00 40.90
ATOM	929	N	ASP A		36.604	51.443	20.897	1.00 29.76
ATOM	930	CA	ASP F		35.585	50.420	20.901	1.00 29.76
ATOM	931	C	ASP F		34.964	50.486	22.309	1.00 29.76
ATOM	932	ō		923	35.466	49.896	23.271	1.00 29.76
ATOM	933	CB	ASP F		36.294	49.081	20.662	1.00100.00
ATOM	934	CG	ASP F		35.357	47.934	20.521	1.00100.00
ATOM	935	OD1			35.131	47.241	21.517	1.00100.00
ATOM	936	OD2	ASP F		34.854	47.713	19.413	1.00100.00
ATOM	938	N	PRO P		33.906	51.274	22,472	1.00 69.79
ATOM	939	CA	PRO P		33.351	51.282	23.821	1.00 69.79
ATOM	940	C	PRO P		32.633	49.968	24.194	1.00 69.79
ATOM	941	ō	PRO P		32.489	49.672	25.371	1.00 69.79
ATOM	942	CB	PRO A		32.449	52.516	23.822	1.00 55.89
ATOM	943	CG	PRO F		32.843	53.260	22.568	1.00 55.89
ATOM	944	CD	PRO F		33.238	52.242	21.601	1.00 55.89
ATOM	945	N	ALA A		32.206	49.183	23.199	1.00100.00
ATOM	946	CA	ALA P		31.555	47.887	23.453	1.00100.00
ATOM	947	C	ALA A		32.501	47.062	24.325	1.00100.00
ATOM	948	0	ALA A		32.137	46.651	25.428	1.00100.00
ATOM	949	CB	ALA A		31.278	47.156	22.146	1.00100.00
MCTA	951	N	PHE P		33.704	46.798	23.809	1.00 39.96
ATOM	952	CA	PHE A		34.714	46.108	24.576	1.00 39.96
ATOM	953	С	PHE A	926	34.808	46.862	25.859	1.00 39.96
ATOM	954	0	PHE A	926	34.279	46.468	26.851	1.00 39.96
ATOM	955	CB	PHE A	926	36.075	46.145	23.886	1.00 99.37
ATOM	956	CG	PHE P	926	37.128	45.350	24.602	1.00 99.37
ATOM	957	CD1	PHE P	926	37.270	43.990	24.365	1.00 99.37
ATOM	958	CD2	PHE P	926	37.940	45.950	25.560	1.00 99.37
ATOM	959	CE1	PHE P	926	38.192	43.248	25.071	1.00 99.37
ATOM	960	CE2	PHE A		38.861	45.217	26.265	1.00 99.37
ATOM	961	CZ	PHE P	926	38.987	43.863	26.023	1.00 99.37
ATOM	963	N	ALA A	927	35.470	47.996	25.823	1.00100.00
ATOM	964	CA	ALA A	927	35.628	48.798	27.018	1.00100.00
ATOM	965	С	ALA A	927	34.627	48.539	28.167	1.00100.00
ATOM	966	0	ALA A		35.030	48.490	29.328	1.00100.00
ATOM	967	CB	ALA A		35.611	50.250	26.619	1.00 37.88
ATOM	969	N	ILE F		33.343	48.348	27.845	1.00 71.50
ATOM	970	CA	ILE A		32.287	48.137	28.866	1.00 71.50
ATOM	971	C	ILE F		31.863	46.700	29.164	1.00 71.50
MOTA	972	0	ILE A		31.579	46.352	30.301	1.00 71.50
ATOM	973	CB	ILE F		30.987	48.939	28.510	1.00 96.87
ATOM	974	CGl	ILE A	928	30.326	49.467	29.787	1.00 96.87

ATOM	975	CG2	ILE A	928	30.008	48.051	27.748	1.00	96.87
ATOM	976	CD1	ILE F	928	28.888	49.846	29.624	1.00	96.87
MOTA	978	N	ALA A		31.793	45.881	28.130	1.00	100.00
ATOM	979	CA	ALA A	929	31.431	44.498	28.319	1.00	100.00
ATOM	980	C	ALA A		32.550	43.917	29.163	1.00	100.00
ATOM	981	0	ALA A		32.326	43.246	30.160	1.00	100.00
ATOM	982	CB	ALA A	929	31.367	43.810	26.982	1.00	31.88
ATOM	984	N	ASN A	930	33.767	44.220	28.737	1.00	37.33
ATOM	985	CA	ASN A	930	35.909	43.775	29.380	1.00	37.33
ATOM	986	C	ASN Z	930	35.326	44.575	30.614	1.00	37.33
ATOM	987	0	ASN A	930	36.020	44.110	31.496	1.00	37.33
ATOM	988	CB	ASN A	930	36.163	43.843	28.378	1.00	87.25
ATOM	989	CG	ASN A	930	36.469	42.497	27.753	1.00	87.25
ATOM	990	OD1	ASN A	. 930	37.485	41.865	28.062	1.00	87.25
ATOM	991	ND2	ASN A	930	35.590	42.051	26.865	1.00	87.25
ATOM	995	N	SER F	931	34.828	45.807	30.629	1.00	35.86
ATOM	996	CA	SER A	931	34.968	46.734	31.740	1.00	35.86
ATOM	997	C	SER A	. 931	36.347	47.321	32.044	1.00	35.86
ATOM	998	0	SER A	931	36.779	47.344	33.211	1.00	35.86
ATOM	999	CB	SER A	931	34.413	46.039	32.992	1.00	47.04
ATOM	1000	OG	SER A	931	34.049	44.700	32.650	1.00	47.04
ATOM	1003	N	THR A	932	37.030	47.813	31.024	1.00	77.19
ATOM	1004	CA	THR A	932	38.346	48.398	31.249	1.00	77.19
ATOM	1005	C	THR A	932	38.655	49.585	30.346	1.00	77.19
ATOM	, 1006	0	THR A	932	38.224	49.632	29.198	1.00	77.19
ATOM	1007	CB	THR P	932	39.453	47.353	31.056	1.00	99.17
ATOM	1008	OG1	THR A	932	39.813	47.299	29.676	1.00	99.17
ATOM	1009	CG2	THR A	932	38.980	45.991	31.492	1.00	99.17
ATOM	1012	N	ALA A		39.376	50.554	30.891	1.00	37.14
ATOM	1013	CA	ALA A		39.814	51.734	30.120	1.00	37.14
ATOM	1014	C	ALA A		40.655	51.286	28.911		37.14
MOTA	1015	0	ALA A	933	40.255	51.495	27.792	1.00	37.14
ATOM	1016	CB	ALA A		40.625	52.743	31.046	1.00	2.00
ATOM	1018	N	SER A		41.814	50.674	29.139	1.00	18.52
ATOM	1019	CA	SER A		42.656	50.117	28.038	1.00	18.52
ATOM	1020	C	SER A		42.578	48.537	27.897	1.00	18.52
ATOM	1021	0	SER A		42.047	47.842	28.815	1.00	18.52
ATOM	1022	CB	SER A		44.114	50.415	28.347	1.00	25.65
ATOM	1023	OG	SER A		44.983	49.645	27.568	1.00	25.65
ATOM	1026	N	THR A	. 935	43.162	48.023	26.794	1.00	63.20
ATOM	1027	CA	THR A		43.338	46.574	26.529	1.00	63.20
ATOM	1028	C	THR A		44.762	46.121	26.957	1.00	63.20
ATOM	1029	O	THR A		45.084	44.947	26.871	1.00	63.20
ATOM	1030	CB	THR A		43.298	46.147	25.069	1.00	29.40
ATOM	1031		THR A		44.470	46.603	24.393	1.00	29.40
ATOM	1032	CG2	THR A		42.095	46.590	24.385		29.40
ATOM	1035	N	LEU A		45.616	47.065	27.349	1.00	6.64
ATOM	1036	CA	LEU A		46.959	46.811	27.861	1.00	6.64
ATOM	1037	C	LEU P		46.654	46.775	29.277	1.00	6.64
MOTA	1038	0	LEU P		45.478	46.916	29.572	1.00	6.64
ATOM	1039	CB	LEU A		47.962	47.919	27.602	1.00	2.00
MOTA	1040	CG	LEU A		48.129	48.224	26.129	1.00	2.00
ATOM	1041		LEU A		48.725	49.731	25.993	1.00	2.00
ATOM	1042		LEU A		48.953	47.147	25.523	1.00	2.00
ATOM	1044	N	SER A		47.638	46.528	30.129	1.00	38.75
ATOM	1045	CA	SER A		47.437	46.434	31.555		38.75
ATOM	1046	C	SER A	937	48.615	47.041	32.342	1.00	38.75

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ATOM	1047	0	SER	71	037	49.664	47.405	31.785	1 00	38.75
		CB	SER			47.257	44.979	31.954		80.09
ATOM	1048		SER				44.274	31.851		80.09
ATOM	1049	OG N	SER			48.471	47.158	33.646		54.88
MOTA	1052	N				48.441				
ATOM	1053	CA	SER			49.489	47.699	34.441		54.88
ATOM	1054	C	SER			50.807	47.155	33.941		54.88
ATOM	1055	0	SER			51.696	47.907	33.571		54.88
ATOM	1056	CB	SER			49.295	47.312	35.887		69.11
ATOM	1057	OG	SER			50.397	47.773	36.631		69.11
ATOM	1060	N	GLN			50.906	45.831	33.902		55.81
ATOM	1061	CA	GLN			52.106	45.148	33.492		55.81
ATOM	1062	C	GLN			52.644	45.445	32.132		55.81
ATOM	1063	0	GLN			53.750	45.896	32.027		55.81
ATOM	1064	CB	GLN			51.924	43.650	33.615		74.76
ATOM	1065	CG	GLN			52.012	43.126	35.014		74.76
ATOM	1066	CD	GLN			53.409	42.973	35.514		74.76
MOTA	1067		GLN			54.238	42.296	34.906		74.76
ATOM	1068	NE2	GLN			53.684	43.597	36.648		74.76
ATOM	1072	N	GLN			51.899	45.176	31.069		26.74
ATOM	1073	CA	GLN			52.446	45.439	29.736		26.74
ATOM	1074	C	GLN			52.963	46.884	29.791		26.74
ATOM	1075	0	GLN			53.929	47.302	29.115		26.74
MOTA	1076	CB	GLN			51.405	45.313	28.639		43.63
MOTA	1077	CG	GLN			51.815	46.080	27.393		43.63
ATOM	1078	CD	GLN			52.444	45.214	26.267		43.63
ATOM	1079		GLN			51.734	44.544	25.479		43.63
ATOM	1080		GLN			53.756	45.236	26.183		43.63
ATOM	1084	И	LEU			52.300	47.595	30.698		30.59
ATOM	1085	CA	TEA			52.514	48.989	30.932		30.59
ATOM	1086	C	LEU			53.800	49.234	31.599		30.59
ATOM	1087	0	LEU			54.611	49.971	31.068		30.59
ATOM	1088	CB	LEU			51.334	49.521	31.709		27.00
ATOM	1089	CG	LEU			50.344	50.390	30.959		27.00
ATOM	1090		LEU			50.253	51.655	31.777		27.00
ATOM	1091	CD2	LEU			50.770	50.642	29.576		27.00
MOTA	1093	N	LEU			53.992	48.683	32.768		26.63
ATOM	1094	CA	LEU			55.284	48.801	33.427		26.63
ATOM	1095	C	LEU		942	56.433	48.144	32.573		26.63
ATOM	1096	0	LEU			57.616	48.326	32.850		26.63
ATOM	1097	CB	LEU			55.208	48.083	34.741	1.00	3.59
ATOM	1098	CG	TEA			55.275	49.016	35.906	1.00	3.59
ATOM	1099		LEU			55.141	48.265	37.321	1.00	3.59
ATOM	1100	CD2	LEU			56.635	49.823	35.675	1.00	3.59
MOTA	1102	N	HIS	А	943	56.084	47.359	31.562		54.79
ATOM	1103	CA	HIS			57.101	46.756	30.741		54.79
ATOM	1104	C	HIS			57.531	47.932	29.905		54.79
MOTA	1105	0	HIS			58.389	48.665	30.324		54.79
MOTA	1106	CB	HIS			56.530	45.638	29.852		38.35
ATOM	1107	CG	HIS			56.799	44.246	30.345		38.35
MOTA	1108		HIS			56.846	43.914	31.682		38.35
ATOM	1109		HIS			56.988	43.092	29.671		38.35
MOTA	1110		HIS			57.050	42.619	31.812		38.35
MCTA	1111	NE2				57.143	42.096	30.603		38.35
MOTA	1115	N			944	56.905	48.115	28.741	1.00	4.19
ATOM	1116	CA			944	57.172	49.217	27.780	1.00	
ATOM	1117	С	PHE	Α	944	58.218	50.257	28.412	1.00	4.19
ATOM	1118	0	PHE	A	944	59.278	50.592	27.781	1.00	4.19

ATOM	1119	CB	PHE	Α	944	55.878	49.913	27.509	1.00	28.23
ATOM	1120	CG	PHE	A	944	55.036	49.255	26.489	1.00	28.23
ATOM	1121	CD1	PHE	А	944	53.632	49.319	26.610		28.23
ATOM	1122	CD2	PHE	Α	944	55.605	48.780	25.336	1.00	
ATOM	1123	CEl	PHE			52.813	48.958	25.614		28.23
ATOM	1124	CE2	PHE			54.769	48.399	24.289		28.23
ATOM	1125	CZ	PHE			53.342	48.504	24.452		28.23
ATOM	1127	N	ALA.			57.874	50.702	29.637		24.23
ATOM	1128	CA	ALA			58.742	51.520	30.434		24.23
ATOM	1129	C	ALA .			59.943	50.648	30.375		24.23
ATOM	1130	0	ALA .			60.623		29.408		24.23
ATOM	1131	CB	ALA .				50.707			
	1133		ALA .			58.270	51.631	31.839		16.89
ATOM		N				60.153	49.775	31.366		23.93
ATOM	1134	CA	ALA .			61.327	48.819	31.493		23.93
ATOM	1135	C	ALA .			62.279	48.525	30.320		23.93
ATOM	1136	0	ALA .			63.460	48.674	30.432		23.93
ATOM	1137	CB	ALA .			60.834	47.495	32.054		76.24
MOTA	1139	N	ASP .			61.796	48.078	29.188	1.00	9.63
ATOM	1140	CA	ASP .			62.727	47.858	28.131	1.00	9.63
ATOM	1141	C	ASP .			63.169	49.132	27.456	1.00	9.63
ATOM	1142	0	ASP .			63.604	49.093	26.290	1.00	9.63
MOTA	1143	CB	ASP .			62.145	46.880	27.114	1.00	
ATOM	1144	CG	ASP .			61.065	47.493	26.259		90.89
MOTA	1145		ASP .			60.143	46.747	25.854	1.00	
ATOM	1146		ASP .			61.128	48.707	25.978		90.89
MOTA	1148	N	VAL .			63.024	50.287	28.098	1.00	60.29
ATOM	1149	CA	VAL .			63.435	51.532	27.459		60.29
ATOM	1150	C	VAL .			64.572	51.963	28.376		60.29
ATOM	1151	0	VAL .			65.604	52.405	27.907		60.29
ATOM	1152	CB	VAL .			62.213	52.606	27.324	1.00	2.00
ATOM	1153		VAL .			62.752	54.133	26.901	1.00	2.00
MOTA	1154		VAL .			61.348	52.297	26.209	1.00	2.00
ATOM	1156	N	ALA .			64.402	51.773	29.686	1.00	12.91
ATOM	1157	CA	ALA.			65.448	52.097	30.677	1.00	
MOTA	1158	C	ALA .			66.681	51.382	30.188		12.91
ATOM	1159	0	ALA .			67.733	52.000	29.956		12.91
MOTA	1160	CB	ALA .			65.135	51.617	32.017	1.00	2.00
ATOM	1162	N	ARG .			66.484	50.078	30.000	1.00	22.64
ATOM	1163	CA	ARG .	A	950	67.422	49.105	29.537	1.00	22.64
ATOM	1164	C	ARG .			68.106	49.588	28.340	1.00	22.64
ATOM	1165	0	ARG	A	950	69.275	49.681	28.386	1.00	22.64
ATOM	1166	CB	ARG .	A	950	66.702	47.783	29.233	1.00	87.27
ATOM	1167	CG	ARG .	A	950	67.146	46.606	30.102	1.00	87.27
ATOM	1168	CD	ARG	A	950	66.806	45.233	29.493	1.00	87.27
ATOM	1169	NE	ARG	Α	950	65.466	45.208	28.912	1.00	87.27
MOTA	1170	CZ	ARG	Α	950	64.341	44.977	29.580	1.00	87.27
ATOM	1171	NHl	ARG	A	950	64.357	44.746	30.879	1.00	87.27
ATOM	1172	NH2	ARG	Α	950	63.188	45.019	28.941	1.00	87.27
ATOM	1179	N	GLY	Α	951	67.435	49.846	27.241	1.00	33.31
MOTA	1180	CA	GLY	Α	951	68.177	50.360	26.102	1.00	33.31
MOTA	1181	C	GLY	Α	951	68.720	51.768	26.462	1.00	33.31
ATOM	1182	0	GLY	A	951	69.514	52.379	25.745	1.00	33.31
ATOM	1184	N	MET	А	952	68.277	52.318	27.588	1.00	48.02
MOTA	1185	CA	MET	Α	952	68.774	53.615	27.949	1.00	48.02
MOTA	1186	C	MET	A	952	70.030	53.440	28.759	1.00	48.02
ATOM	1187	0	MET	A	952	70.861	54.316	28.719	1.00	48.02
ATOM	1188	CB	MET	A	952	67.721	54.442	28.720	1.00	58.75

3.mov	1189	CG	MET	70	952	67.277	55.792	28.089	1.00	58.75
ATOM					952	67.797	56.265	26.390		58.75
MOTA	1190	SD	MET			69.079	57.471	26.826		58.75
ATOM	1191	CE					52.325	29.494		30.83
ATOM	1193	N	ASP			70.145	51.942	30.317		30.83
ATOM	1194	CA	ASP			71.299				30.83
MOTA	1195	C			953	72.393	51.689	29.346		30.83
MOTA	1196	0			953	73.521	52.078	29.523		
ATOM	1197	CB	ASP			71.084	50.617	30.955		30.69
ATOM	1198	CG	ASP			71.512	50.589	32.381		30.69
ATOM	1199	ODl	ASP			71.504	51.661	32.997		30.69
ATOM	1200	OD2	ASP	Α	953	71.838	49.485	32.907		30.69
ATOM	1202	N	TYR	Α	954	72.031	50.999	28.292		19.34
ATOM	1203	CA	TYR	A	954	72.952	50.630	27.239	1.00	19.34
ATOM	1204	C	TYR	Α	954	73.559	51.896	26.762	1.00	19.34
ATOM	1205	0	TYR	Α	954	74.529	52.327	27.362	1.00	19.34
ATOM	1206	CB	TYR	A	954	72.236	49.887	26.117	1.00	37.26
ATOM	1207	CG	TYR	A	954	73.181	49.115	25.244	1.00	37.26
ATOM	1208	CD1	TYR			74.158	48.238	25.784	1.00	37.26
ATOM	1209	CD2	TYR		954	73.149	49.300	23.871	1.00	37.26
ATOM	1210	CE1	TYR		954	75.072	47.594	24.942	1.00	37.26
ATOM	1211	CE2	TYR			74.042	48.676	23.041	1.00	37.26
ATOM	1212	CZ	TYR			74.993	47.843	23.568	1.00	37.26
ATOM	1212	OH	TYR			75.859	47.367	22.645		37.26
	1216	N	LEU			72.967	52.501	25.722		49.71
ATOM		CA	LEU			73.404	53.781	25.150		49.71
MOTA	1217	C	LEU			73.404	54.641	26.293		49.71
ATOM	1218						55.109	26.279		49.71
ATOM	1219	0	LEU			74.950	54.530	24.439	1.00	17.74
MOTA	1220	CB	LEU				53.937	23.292	1.00	17.74
ATOM	1221	CG	LEU			71.456		23.292	1.00	
MOTA	1222	CD1	LEU		955	69.972	54.493	21.914		17.74
ATOM	1223	CD2	LEU			71.989	54.345	27.293		34.64
MOTA	1225	N			956	73.012	54.840	28.404	1.00	34.64
ATOM	1226	CA			956	73.430	55.663			34.64
ATOM	1227	C			956	74.843	55.360	28.778		34.64
ATOM	1228	0	SER		956	75.701	56.218	28.579	1.00	
ATOM	1229	CB			956	72.561	55.495	29.622	1.00	37.38
ATOM	1230	OG			956	73.071	56.228	30.699	1.00	
MOTA	1233	N			957	75.134	54.188	29.321		33.59
ATOM	1234	CA			957	76.511	53.895	29.680		33.59
ATOM	1235	C	GLN	Α	957	77.379	53.837	28.410		33.59
ATOM	1236	0	GLN	A	957	77.719	52.798	27.943		33.59
ATOM	1237	CB	GLN	Α	957	76.583	52.568	30.455		42.10
ATOM	1238	CG			957	76.621	52.721	32.002		42.10
ATOM	1239	CD	GLN	Α	957	77.483	53.951	32.500		42.10
ATOM	1240	OE1	GLN	Α	957	78.321	54.499	31.739		42.10
ATOM	1241	NE2	GLN	Α	957	77.274	54.367	33.780		42.10
ATOM	1245	N	LYS	Α	958	77.739	54.952	27.823		99.18
ATOM	1246	CA	LYS	A	958	78.543	54.854	26.620	1.00	99.18
ATOM	1247	C			958	78.688	56.227	26.039	1.00	
ATOM	1248	ō			958	79.111	56.370	24.897	1.00	99.18
ATOM	1249	CB			958	77.880	53.934	25.586	1.00	99.74
ATOM	1250	CG			958	78.545	52.582	25.404	1.00	99.74
ATOM	1251	CD	LYS		958	77.830	51.738	24.360	1.00	99.74
ATOM	1252	CE			958	77.997	50.238	24.629	1.00	99.74
ATOM	1252	NZ			958	78.459	49.456	23.434	1.00	
ATOM	1253	N			. 959	78.327	57.233	26.832	1.00	
ATOM	1259	CA			959	78.423	58.615	26.402	1.00	
ALUM	1723	UP4	2777		د د د د	10.423	50.025	2.1.100		

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Title: Method of Identifying Inhibitors of TIE-2 Inventors: Nancy J. Bump *et al.*

ATOM	1260	C	GLN	A	959	77.378	58.947	25.376	1.00	73.45
ATOM	1261	0	GLN	А	959	77.493	59.970	24.702	1.00	
ATOM	1262	CB	GLN	Α	959	79.785	58.882	25.784	1.00	
ATOM	1263	CG	GLN	Α	959	80.899	58.069	26.399	1.00	19.35
ATOM	1264	CD	GLN	Α	959	80.957	58.449	27.805	1.00	19.35
ATOM	1265	OE1				80.252	59.453	28.221	1.00	19.35
ATOM	1266	NE2	GLN			81.763	57.708	28.610	1.00	19.35
ATOM	1270	N			960	76.376	58.075	25.242		
ATOM	1271	CA			960	75.312	58.292	24.262	1.00	36.08
ATOM	1272	C			960	74.223			1.00	
ATOM	1273	0			960		59.102	24.958	1.00	36.08
ATOM	1274	CB				73.754	58.762	26.078	1.00	
ATOM	1275	CG			960	74.810	56.957	23.718	1.00	
					960	75.670	56.407	22.614		85.11
ATOM	1276		PHE			76.531	55.349	22.839		85.11
ATOM	1277	CD2	PHE			75.656	56.981	21.350		85.11
ATOM	1278	CE1	PHE			77.361	54.879	21.822	1.00	85.11
ATOM	1279	CE2	PHE			76.493	56.505	20.330	1.00	85.11
ATOM	1280	CZ			960	77.338	55.461	20.572	1.00	85.11
ATOM	1282	N	ILE	Α	961	73.918	60.227	24.300	1.00	30.22
ATOM	1283	CA	ILE	Α	961	72.939	61.196	24.749	1.00	30.22
MOTA	1284	C	ILE	Α	961	71.858	61.213	23.713		30.22
MOTA	1285	0	ILE	Α	961	72.112	61.420	22.545		30.22
MOTA	1286	CB	ILE	Α	961	73.536	62.578	24.911	1.00	71.39
ATOM	1287	CG1	ILE			74.693	62.526	25.899		71.39
ATOM	1288	CG2	ILE			72.488	63.518	25.442		71.39
ATOM	1289		ILE			75.888	63.302	25.476		71.39
ATOM	1291	N	HIS			70.627	61.034	24.158		
ATOM	1292	CA	HIS			69.524	60.924			80.58
ATOM	1293	C	HIS			68.798		23.236		80.58
ATOM	1294	ō	HIS			69.179	62.196	22.692	1.00	80.58
ATOM	1295	CB	HIS				62.676	21.629	1.00	80.58
ATOM	1295	CG	HIS			68.584	59.904	23.855	1.00	39.42
ATOM	1290					67.415	59.585	23.008	1.00	39.42
					962	67.142	58.316	22.575	1.00	39.42
ATOM	1298	CD2	HIS			66.450	60.378	22.499	1.00	39.42
ATOM	1299	CE1			962	66.052	58.335	21.832	1.00	39.42
ATOM	1300	NE2			962	65.617	59.580	21.772	1.00	39.42
ATOM	1304	N	ARG		963	67.745	62.694	23.367	1.00	25.62
ATOM	1305	CA	ARG			67.008	63.920	22.979	1.00	25.62
MOTA	1306	C	ARG		963	65.777	63.852	22.084	1.00	25.62
ATOM	1307	0	ARG		963	65.762	64.331	20.941	1.00	25.62
ATOM	1308	CB	ARG		963	67.977	64.955	22.380	1.00	98.75
ATOM	1309	CG	ARG	Α	963	69.318	65.061	23.081	1.00	98.75
ATOM	1310	CD	ARG	А	963	70.230	66.016	22.356	1.00	98.75
ATOM	1311	NE	ARG	A	963	70.718	65.501	21.087	1.00	98.75
ATOM	1312	CZ	ARG	Α	963	70.212	65.832	19.911	1.00	98.75
ATOM	1313	NH1	ARG	Α	963	69.200	66.680	19.852	1.00	98.75
ATOM	1314	NH2	ARG	Α	963	70.717	65.321	18.801		98.75
ATOM	1321	N	ASN	А	964	64.738	63.276	22.661	1.00	47.91
ATOM	1322	CA	ASN		964	63.442	63.070	22.035		47.91
ATOM	1323	C	ASN			63.235	61.618	22.246		47.91
ATOM	1324	0	ASN			63.068	60.856	21.302		
ATOM	1325	CB			964	63.453	63.377			47.91
ATOM	1326	CG	ASN		964			20.538	1.00	84.77
ATOM	1327		ASN			62.453	54.459	20.153	1.00	34.77
ATOM					964	61.509	64.768	20.902		84.77
	1328				964	62.653	65.039	18.977	1.00	84.77
ATOM	1332	N	LEU		965	63.366	61.249	23.509	1.00	96.70
MOTA	1333	CA	LEU	A	965	63.1481	59.897	23.937	1.00	96.70

ATOM	1334	C	LEU	Α	965	61.836	60.220	24.659	1.00 96.70
MOTA	1335	0	LEU	A	965	61.784	60.527	25.833	1.00 96.70
ATOM	1336	CB	LEU	Α	965	64.352	59.382	24.805	1.00 17.46
ATOM	1337	CG	LEU	А	965	64.456	58.589	26.099	1.00 17.46
ATOM	1338		LEU			65.774	58.784	26.891	1.00 17.46
ATOM	1339	CD2	LEU			63.423	59.114	26.967	1.00 17.46
ATOM	1341	N	ALA			60.794	60.283	23.833	1.00 71.46
ATOM	1342	CA	ALA			59.408	60.534	24.219	1.00 71.46
ATOM	1343	C	ALA			58,601	59.518	24.219	
ATOM	1344	0	ALA						
						59.009	59.122	22.314	1.00 71.46
ATOM	1345	CB	ALA			59.005	61.933	23.885	1.00 62.29
ATOM	1347	14	ALA			57.457	59.105	23.908	1.00 34.40
MOTA	1348	CA	ALA			56.641	58.086	23.249	1.00 34.40
MOTA	1349	C	ALA			56.585	58.066	21.726	1.00 34.40
ATOM	1350	0	ALA			56.689	57.011	21.106	1.00 34.40
ATOM	1351	CB	ALA	А	967	55.236	58.088	23.807	1.00 31.96
MOTA	1353	1/1	ARG	Α	968	56.462	59.208	21.094	1.00 9.59
ATOM	1354	CA	ARG	Α	968	56.309	59.113	19.678	1.00 9.59
ATOM	1355	C	ARG	Α	968	57.467	58.532	19.054	1.00 9.59
ATOM	1356	0	ARG	Α	968	57.335	58.106	17.930	1.00 9.59
ATOM	1357	CB	ARG			55.960	60.480	19.013	1.00 12.36
ATOM	1358	CG	ARG			56.480	61.806	19.751	1.00 12.36
ATOM	1359	CD	ARG			56.426	62.907	18.727	1.00 12.36
ATOM	1360	NE	ARG			57.453	63.898	18.879	1.00 12.36
ATOM	1361	CZ	ARG			57.608	64.568	19.994	1.00 12.36
ATOM	1362	NH1	ARG			56.746		20.994	1.00 12.36
		NH2	ARG				64.307		
ATOM	1363					58.718	65.297	20.206	1.00 12.36
ATOM	1370	N	ASN			58.611	58.550	19.735	1.00 56.22
ATOM	1371	CA	ASN			59.878	58.043	19.179	1.00 56.22
ATOM	1372	С	ASN			60.309	56.672	19.730	1.00 56.22
ATOM	1373	0	ASN			61.472	56.327	19.673	1.00 56.22
MOTA	1374	CB	ASN			61.011	59.053	19.444	1.00 99.68
ATOM	1375	CG	ASN	А	969	60.674	60.482	18.998	1.00 99.68
ATOM	1376	ODl	ASN	Α	969	60.213	61.303	19.787	1.00 99.68
MOTA	1377	ND2	ASN	А	969	60.926	60.780	17.732	1.00 99.68
ATOM	1381	N	ILE	A	970	59.351	55.935	20.288	1.00 10.68
ATOM	1382	CA	ILE	A	970	59.507	54.683	20.853	1.00 10.68
ATOM	1383	C	ILE	Α	970	58.651	53.708	20.079	1.00 10.68
ATOM	1384	0	ILE	A	970	57.450	53.865	20.060	1.00 10.68
MOTA	1385	CB	ILE	А	970	59.003	54.602	22.168	1.00 11.62
ATOM	1386	CG1	ILE			59.808	55.496	23.084	1.00 11.62
ATOM	1387	CG2	ILE			59.191	53.056	22.620	1.00 11.62
ATOM	1388	CD1	ILE			61.263	55.730	22.600	1.00 11.62
ATOM	1390	N			971	59.250	52.676	19.496	1.00 31.69
ATOM		CA			971				
	1391					58.518	51.699	18.733	
ATOM	1392	C	LEU			58.148	50.357	19.369	1.00 31.69
ATOM	1393	0	LEU			58.938	49.792	20.148	1.00 31.69
ATOM	1394	CB			971	59.308	51.333	17.535	1.00 17.23
ATOM	1395	CG	LEU		971	59.702	52.411	16.632	1.00 17.23
ATOM	1396	CD1	LEU		971	60.981	51.973	16.005	1.00 17.23
ATOM	1397	CD2	LEU		971	58.629	52.642	15.646	1.00 17.23
MOTA	1399	N			972	56.953	49.832	19.017	1.00 20.91
ATOM	1400	CA			972	56.655	48.486	19.475	1.00 20.91
ATOM	1401	C	VAL	А	972	56.862	47.491	18.389	1.00 20.91
ATOM	1402	0	VAL	A	972	56.022	47.375	17.523	1.00 20.91
ATOM	1403	CB	VAL	Α	972	55.344	48.349	19.953	1.00 9.13
ATOM	1404		VAL	A	972	55.362	47.291	21.081	1.00 9.13

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ATOM	1405	CG2	VAL	A	972	54.797	49.894	20.467	1.00 9.13
ATOM	1407	N	GLY	Α	973	58.077	46.873	18.414	1.00 32.46
ATOM	1408	CA	GLY	A	973	58.514	45.851	17.466	1.00 32.46
ATOM	1409	C	GLY	Α	973	58.012	44.434	17.814	1.00 32.46
ATOM	1410	0	GLY	Α	973	57.324	44.254	18.816	1.00 32.46
ATOM	1412	N	GLU	А	974	58.393	43.403	17.055	1.00 22.44
ATOM	1413	CA	GLU	A	974	57.845	42.109	17.351	1.00 22.44
ATOM	1414	C	GLU .			57.902	41.725	18.793	1.00 22.44
ATOM	1415	ō	GLU		974	58.809	42.041	19.510	1.00 22.44
ATOM	1416	CB	GLU			58.364	41.035	16.394	1.00 65.78
ATOM	1417	CG	GLU		974	57.385	40.798	15.138	1.00 65.78
ATOM	1418	CD	GLU .		974	55.821	40.585	15.469	1.00 65.78
ATOM	1419	OE1	GLU			55.398	40.463	16.656	1.00 65.78
ATOM	1420	OE2	GLU			55.005	40.540	14.512	1.00 65.78
ATOM	1422	N	ASN			56.767	41.210	19.246	1.00 22.08
ATOM	1423	CA	ASN			56.540	40.717	20.627	1.00 22.08
ATOM	1424	C	ASN			56.037	41.756	21.638	1.00 22.08
ATOM	1425	ō	ASN .			55.968	41.482	22.844	1.00 22.08
ATOM	1426	CB	ASN .			57.810	40.016	21.140	1.00 99.25
ATOM	1427	CG	ASN .			58.074	38.679	20.438	1.00 99.25
ATOM	1428	OD1	ASN .			58.836	37.859	20.929	1.00 99.25
ATOM	1429	ND2	ASN .			57.446	38.465	19.292	1.00 99.25
ATOM	1433	N	TYR .			55.656	42.932	21.134	1.00 30.29
ATOM	1434	CA	TYR			55.204	44.013	21.134	1.00 30.29
ATOM	1435	C	TYR			56.427	44.631	22.697	1.00 30.29
ATOM	1436	0	TYR .			56.331	45.214	23.759	1.00 30.29
ATOM	- 1437	CB	TYR .				43.463	22.893	1.00 30.29
ATOM	1438	CG	TYR .			54.157			
ATOM	1438	CD1	TYR .			53.001	42.961	22.089	1.00 71.60
		CD2	TYR.			52.698	41.611	22.036	
ATOM ATOM	1440	CEI	TYR			52.229	43.840	21.339	1.00 71.60
ATOM	1441	CE2	TYR .			51.652	41.145		
ATOM		CZ				51.181	43.390	20.547	1.00 71.60
	1443		TYR			50.895	42.043	20.491	1.00 71.60
ATOM	1444	OH	TYR.			49.905	41.588	19.655	1.00 71.60
ATOM	1447	N	VAL .			57.569	44.513	22.047	1.00 35.58
ATOM	1448	CA	VAL			58.837	44.988	22.597	1.00 35.58
ATOM	1449	C	VAL			59.247	46.367	22.101	1.00 35.58
ATOM	1450	0	VAL.			59.495	46.616	20.903	1.00 35.58
ATOM	1451	CB	VAL			59.994	43.975	22.316	1.00 54.29
ATOM	1452	CG1	VAL			61.110	44.134	23.340	1.00 54.29
ATOM	1453	CG2	VAL			59.418	42.533	22.339	1.00 54.29
ATOM	1455	N	ALA			59.355	47.233	23.082	1.00 36.83
MOTA	1456	CA	ALA			59.628	48.594	22.857	1.00 36.83
MOTA	1457	C	ALA			61.086	49.005	22.550	1.00 36.83
ATOM	1458	0	ALA			61.937	48.823	23.380	1.00 36.83
MOTA	1459	CB	ALA			59.142	49.265	24.019	1.00 27.14
MOTA	1461	N	LYS			61.368	49.570	21.374	1.00 42.93
MOTA	1462	CA	LYS			62.704	50.023	21.063	1.00 42.93
MOTA	1463	С	LYS			63.002	51.530	20.907	1.00 42.93
MOTA	1464	0	LYS			62.175	52.352	20.414	1.00 42.93
ATOM	1465	CB	LYS			63.190	49.433	19.798	1.00 32.23
MOTA	1466	CG	LYS			62.273	48.708	19.039	1.00 32.23
ATOM	1467	CD	LYS			62.556	47.230	19.416	1.00 32.23
MOTA	1468	CE	LYS	A	979	63.156	46.356	18.275	1.00 32.23
ATOM	1469	ΝZ	LYS	Α	979	63.744	45.144	18.883	1.00 32.23
ATOM	1474	N	ILE	A	980	64.233	51.887	21.275	1.00 2.00
ATOM	1475	CA	ILE	Α	980	64.639	53.265	21.099	1.00 2.00

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ATOM	1476	С	TID	7.	980	65.044	53.446	19.649	1 00 0 00
ATOM	1477	0			980	65.191	52.445	18.913	1.00 2.00
ATOM	1478	CB	ILE			65.717	53.649		
ATOM	1479	CG1	ILE			65.318	53.372	22.019	1.00 22.25
ATOM	1480	CG2	ILE			65.839	55.073	21.885	1.00 22.25
ATOM	1481	CD1	ILE			66.358	53.040	24.467	1.00 22.25
ATOM	1483	N	ALA		981	65.129	54.715	19.235	1.00 22.25
ATOM	1484	CA	ALA		981	65.489	55.166	17.870	1.00 37.10
ATOM	1485	C	ALA			65.426	56.684	17.652	1.00 37.10
ATOM	1486	Ö	ALA		981	64.905	57.454	18.494	1.00 37.10
ATOM	1487	CB	ALA		981	64.634	54.620	16.964	1.00 37.10
ATOM	1489	N		A	982	65.933	57.120	16.508	1.00 12.10
ATOM	1490	CA	ASP		982	65.907	58.525	16.186	1.00 81.89
ATOM	1491	C	ASP		982	66.821	59.190	17.201	1.00 81.89
ATOM	1492	0	ASP	A	982	66.877	60.416	17.342	1.00 81.89
ATOM	1493	CB		A	982	64.465	59.029	16.284	1.00 22.36
ATOM	1494	CG	ASP		982	64.352	60.357	16.999	1.00 22.36
ATOM	1495		ASP		982	64.517	61.390	16.281	1.00 22.36
MOTA	1496	OD2	ASP	Ā	982	64.112	60.353	18.252	1.00 22.36
ATOM	1498	N			983	67.540	58.353	17.922	1.00 90.03
ATOM	1499	CA			983	68.502	58.819	18.897	1.00 90.03
ATOM	1500	C	PHE		983	69.521	59.638	18.083	1.00 90.03
ATOM	1501	Ö	PHE	A	983	69.436	59.728	16.844	1.00 90.03
ATOM	1502	CB			983	69.205	57.599	19.489	1.00100.00
ATOM	1503	CG	PHE		983	69.417	56.489	18.475	1.00100.00
ATOM	1504	CD1	PHE		983	70.419	56.593	17.502	1.00100.00
ATOM	1505	CD2	PHE	A	983	68.567	55.387	18.435	1.00100.00
ATOM	1506	CE1	PHE		983	70.557	55.624	16.513	1.00100.00
ATOM	1507	CE2			983	68.704	54.418	17.449	1.00100.00
ATOM	1508	CZ	PHE		983	69.698	54.537	16.488	1.00100.00
ATOM	1510	N			984	70.493	60.226	18.770	1.00 59.78
ATOM	1511	CA			984	71.533	60.957	18.060	1.00 59.78
ATOM	1512	Ċ	GLY	A	984	72.821	60.159	18.193	1.00 59.78
ATOM	1513	0		A	984	72.900	59.221	19.019	1.00 59.78
ATOM	1515	N	LEU		985	73.816	60.488	17.379	1.00 99.32
ATOM	1516	CA	LEU	А	985	75.094	59.791	17.454	1.00 99.32
ATOM	1517	C	LEU		985	75.886	60.603	18.440	1.00 99.32
ATOM	1518	0	LEU	A	985	77.068	60.348	18.669	1.00 99.32
ATOM	1519	CB			985	75.824	59.786	16.106	1.00100.00
ATOM	1520	CG	LEU	А	985	75.453	58.753	15.036	1.00100.00
MOTA	1521	CD1	LEU	Α	985	74.707	57.590	15.651	1.00100.00
ATOM	1522	CD2	LEU	А	985	74.604	59.428	13.971	1.00100.00
ATOM	1524	N	SER	A	986	75.211	61.587	19.020	1.00 37.75
MOTA	1525	CA	SER	А	986	75.828	62.476	19.989	1.00 37.75
ATOM	1526	С	SER	Α	986	76.413	61.806	21.210	1.00 37.75
ATOM	1527	0	SER	Α	986	75.708	61.541	22.143	1.00 37.75
ATOM	1528	CB	SER	A	986	74.830	63.525	20.445	1.00 99.91
ATOM	1529	OG	SER	Α	986	75.198	64.776	19.917	1.00 99.91
ATOM	1532	N	ARG	A	987	77.710	61.513	21.216	1.00 63.13
ATOM	1533	CA	ARG	Α	987	78.285	60.910	22.407	1.00 63.13
MOTA	1534	C	ARG	Α	987	79.243	61.904	22.979	1.00 63.13
ATOM	1535	0	ARG	Α	987	80.058	62.476	22.270	1.00 63.13
ATOM	1536	CB	ARC	A	987	78.964	59.567	22.132	1.00 87.40
ATOM	1537	CG	ARG	Α	987	79.870	59.529	20.947	1.00 87.40
ATOM	1538	CD	ARG	Α	987	81.110	58.722	21.273	1.00 87.40
MOTA	1539	NE	ARG	Α	987	80.807	57.654	22.217	1.00 87.40
ATOM	1540	CZ	ARG	A	987	80.782	56.366	21.898	1.00 87.40

ATOM 1541 NH1 ARG A 987 81.042 55.981 20.658 1.00 87.40 ATOM 1542 NH2 ARG A 987 80.506 55.463 22.824 1.00 87.40 ATOM 1549 N GLY A 988 79.090 62.096 24.282 1.00 28.62 ATOM 1550 CA GLY A 988 79.833 63.044 25.072 1.00 28.62 ATOM 1542 NH2 ARG A 987 80.502 55.463 22.824 1.00 87.40 ATOM 1549 N GLY A 988 79.090 62.096 24.282 1.00 87.40 ATOM 1551 C GLY A 988 79.833 63.044 25.072 1.00 28.62 ATOM 1551 C GLY A 988 79.833 63.044 25.072 1.00 28.62 ATOM 1552 O GLY A 988 79.838 662.156 26.816 1.00 28.62 ATOM 1554 N GLN A 989 79.268 63.073 26.476 1.00 28.62 ATOM 1554 O GLN A 989 79.268 62.156 26.816 1.00 22.70 ATOM 1555 CA GLN A 989 79.612 64.094 27.270 1.00 22.70 ATOM 1557 O GLN A 989 79.612 64.094 27.270 1.00 22.70 ATOM 1558 CB GLN A 989 80.449 64.672 29.785 1.00 22.70 ATOM 1558 CB GLN A 989 80.449 64.672 29.785 1.00 22.70 ATOM 1558 CB GLN A 989 80.449 64.672 29.785 1.00 22.70 ATOM 1556 DC GLN A 989 81.276 65.539 31.644 1.00 98.73 ATOM 1560 CD GLN A 989 81.240 66.722 31.049 1.00 98.73 ATOM 1560 CD GLN A 989 81.240 66.722 31.049 1.00 98.73 ATOM 1561 DEI GLN A 990 77.173 67.478 27.725 1.00 98.73 ATOM 1562 NEZ GLN A 990 77.173 67.478 27.725 1.00 47.13 ATOM 1567 CA GLU A 990 77.106 67.842 25.251 1.00 47.13 ATOM 1569 O GLU A 990 77.106 67.842 25.251 1.00 47.13 ATOM 1569 O GLU A 990 77.106 67.842 25.255 1.00 47.13 ATOM 1570 CB GLU A 990 77.930 68.612 28.534 1.00 77.23 ATOM 1570 CB GLU A 990 77.930 68.612 28.534 1.00 77.23 ATOM 1570 CB GLU A 990 77.830 68.612 28.534 1.00 77.23 ATOM 1570 CB GLU A 990 77.830 68.612 28.534 1.00 77.23 ATOM 1570 CB GLU A 990 77.830 68.612 28.534 1.00 77.23 ATOM 1570 CB GLU A 990 77.830 68.612 28.534 1.00 77.23 ATOM 1570 CB GLU A 990 77.830 68.612 28.534 1.00 77.23 ATOM 1570 CB GLU A 990 77.830 68.612 28.534 1.00 77.23 ATOM 1570 CB GLU A 990 77.830 68.612 28.534 1.00 77.23 ATOM 1570 CB GLU A 990 77.830 68.612 28.534 1.00 77.23 ATOM 1570 CB GLU A 990 77.830 68.612 28.534 1.00 77.23 ATOM 1570 CB GLU A 990 77.830 68.612 28.534 1.00 77.23 ATOM 1570 CB GLU A 990 77.830 68.612 28.534 1.00 77.23 ATOM 1570 CB GLU A 990 77.437 69.869 28.704 1.00 24.20 ATOM 1570 CB GLU A 990 77.437 69.869 28.704 1.00 24.20 ATOM 1570 CB GLU A 990 77.437 69.869 28.704 1.00 24.20 ATOM 1570 CB GLU A 990 77.437 69.869 28.704 1.00 24.20 ATOM 1570 CB GLU

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ATOM	1613	CE		A 994	70.	694	80.150	18.153	1.001	100.00
ATOM	1614	NZ	LYS	A 994	71.	425	81.159	18.962	1.001	100.00
ATOM	1619	N	LYS	A 995	68.	446	75.287	17.488	1.00	66.77
ATOM	1620	CA	LYS	A 995	67.	741	75.142	16.210	1.00	66.77
ATOM	1621	C	LYS	A 995	68.	023	73.749	15.591	1.00	66.77
ATOM	1622	0	LYS	A 995	67.	910	73.583	14.358	1.00	66.77
ATOM	1623	CB	LYS	A 995	68.	167	76.265	15.244	1.001	.00.00
ATOM	1624	OXT	LYS	A 995	68.	354	72.815	16.355	1.001	.00.00
ATOM	1626	N	PRO	A1001	61.	032	69.682	22.189	1.00	23.57
ATOM	1627	CA	PRO	A1001	59.	754	69.092	22.679	1.00	23.57
ATOM	1628	C	PRO	A1001	59.	681	69.765	24.004	1.00	23.57
ATOM	1629	0	PRO	A1001	59.	857	69.162	25.026	1.00	23.57
ATOM	1630	CB	PRO	A1001	59.	964	67.607	22.863	1.00	82.24
ATOM	1631	CG	PRO	A1001	61.	529	67.446	22.804	1.00	82.24
ATOM	1632	CD	PRO	A1001	62.	179	68.812	22.494	1.00	82.24
ATOM	1635	N	VAL	A1002	59.	429	71.067	23.965	1.00	14.96
ATOM	1636	CA	VAL	A1002	59.	401	71.905	25.163	1.00	14.96
ATOM	1637	C	VAL	A1002	58.	731	71.247	26.277	1.00	14.96
ATOM	1638	0	VAL	A1002	58.	930	71.607	27.409	1.00	14.96
ATOM	1639	CB	VAL	A1002	58.	755	73.268	24.833	1.00	66.63
ATOM	1640	CG1	VAL	A1002	57.	691	73.065	23.764	1.00	66.63
ATOM	1641	CG2	VAL	A1002	58.	212	73.946	26.088	1.00	66.63
ATOM	1643	N	ARG	A1003	57.	913	70.256	25.990	1.00	36.10
ATOM	1644	CA	ARG	A1003	57.	188	69.580	27.054	1.00	36.10
ATOM	1645	C	ARG	A1003	57.	957	68.409	27.649	1.00	36.10
ATOM	1646	0	ARG	A1003	57.	762	68.012	28.773	1.00	36.10
ATOM	1647	CB	ARG	A1003	55.	829	69.195	26.507	1.00	97.10
ATOM	1648	CG	ARG	A1003	55.	381	70.237	25.495	1.00	97.10
ATOM	1649	CD	ARG	A1003	53.	974	70.007	25.036	1.00	97.10
ATOM	1650	NE	ARG	A1003	53.	022	70.432	26.045	1.00	97.10
ATOM	1651	CZ	ARG	A1003	51.	949	71.153	25.782	1.00	97.10
ATOM	1652	NH1	ARG	A1003	51.	699	71.527	24.544	1.00	97.10
ATOM	1653	NH2	ARG	A1003	51.	136	71.493	26.759	1.00	97.10
ATOM	1660	N	TRP	A1004	58.	902	67.934	26.865	1.00	31.39
ATOM	1661	CA	TRP	A1004	59.	799	66.858	27.231	1.00	31.39
MOTA	1662	С	TRP	A1004	61.	031	67.342	27.941	1.00	31.39
ATOM	1663	0	TRP	A1004	61.	431	66.841	28.992	1.00	31.39
MOTA	1664	CB	TRP	A1004	60.	117	66.113	25.981	1.00	37.57
ATOM	1665	CG	TRP	A1004	59.	058	65.128	25.860	1.00	37.57
ATOM	1666	CD1	TRP	A1004	59.	055	63.870	26.415	1.00	37.57
ATOM	1667	CD2	TRP	A1004	57.	758	65.324	25.323	1.00	37.57
ATOM	1668	NE1	TRP	A1004	57.	832	63.290	26.253	1.00	37.57
ATOM	1669	CE2	TRP	A1004	57.	011	64.149	25.594	1.00	37.57
ATOM	1670	CE3	TRP	A1004	57.	142	66.370	24.648	1.00	37.57
ATOM	1671	CZ2	TRP	A1004	55.	683	63.991	25.214	1.00	37.57
ATOM	1672	CZ3	TRP	A1004	55.	789	66.223	24.252	1.00	37.57
ATOM	1673	CH2	TRP	A1004	55.	087	65.041	24.541	1.00	37.57
ATOM	1676	3/2	MET	A1005	61.	556	68.426	27.391	1.00	10.72
ATOM	1677	CA	MET	A1005		723	69.067	27.879	1.00	10.72
ATOM	1678	C	MET	A1005		709	69.405	29.340	1.00	10.72
ATOM	1679	0	MET	A1005		690	69.822	29.947	1.00	10.72
ATOM	1680	CB	MET	A1005		983	70.254	27.003	1.00	63.30
MOTA	1681	CG	MET	A1005		299	69.783	25.632	1.00	
MOTA	1682	SD	MET	A1005		194	71.078	24.467	1.00	
ATOM	1683	CE	MET	A1005		494	72.111	25.002	1.00	63.30
ATOM	1685	N		A1006		873	69.180	29.939		13.71
ATOM	1686	CA	ALA	A1006		092	69.541	31.343	1.00	13.71

ATOM	1687	C		A1006	64.634	71.015	31.321	1.00	13.71
MOTA	1688	0		A1006	64.885	71.575	30.254	1.00	
ATOM	1689	CB	ALA	A1006	65.114	68.618	31.976		44.23
ATOM	1691	N	ILE	A1007	64.762	71.597	32.515	1.00	21.54
ATOM	1692	CA	ILE	A1007	65.278	72.951	32.738		21.54
ATOM	1693	C	ILE	A1007	66.586	73.324	31.943		21.54
ATOM	1694	0	ILE	A1007	66.528	73.791	30.817		21.54
ATOM	1695	CB	ILE	A1007	65.482	73.137	34.300		20.90
ATOM	1696	CG1	ILE	A1007	66.672	72.188	34.830		20.90
ATOM	1697	CG2	ILE	A1007	64.088	72.800	35.034		20.90
ATOM	1698	CD1		A1007	67.395	72.474	36.237		20.90
ATOM	1700	N	GLU	A1008	67.752	73.082	32.510	1.00	
ATOM	1701	CA		A1008	69.028	73.410	31.892		10.72
ATOM	1702	C		A1008	69.066	73.404	30.369	1.00	
ATOM	1703	ō		A1008	70.144	73.771	29.757	1.00	
ATOM	1704	CB		A1008	70.144	72.429			10.72
ATOM	1705	CG		A1008	69.942	70.977	32.417	1.00	
ATOM	1706	CD		A1008	69.159		31.916		39.30
ATOM	1707	OE1		A1008		70.091	32.896		39.30
ATOM	1708	OE2		A1008	68.082	70.549	33.382		39.30
ATOM	1710	N		A1009	69.634	68.944	33.178		39.30
ATOM	1711	CA			67.976	72.880	29.764		31.45
ATOM	1712	CA		A1009	67.798	72.791	28.314		31.45
ATOM				A1009	66.826	73.844	27.779		31.45
ATOM	1713	0		A1009	67.007	74.396	26.685		31.45
ATOM	1714	CB		A1009	67.286	71.410	27.930		100.00
ATOM	1715	OG		A1009	68.088	70.402	28.500		100.00
	1718	N		A1010	65.745	74.095	28.485		75.06
ATOM ATOM	1719	CA		A1010	64.852	75.103	27.977		75.06
ATOM	1720 1721	C		A1010	65.758	76.342	27.926		75.06
ATOM	1722	CB		A1010	65.737	77.146	26.989		75.06
ATOM				A1010	63.675	75.238	28.938		62.28
ATOM	1723	CG		A1010	62.685	74.078	28.725		62.28
ATOM	1724 1725	CD1		A1010	61.421	74.394	29.511		62.28
ATOM	1725	CD2		A1010	62.379	73.854	27.229		
		N		A1011	66.597	76.401	28.951		36.75
MOTA	1728	CA		A1011	67.611	77.389	29.207		36.75
ATOM	1729	C		A1011	68.761	77.280	28.189		36.75
ATOM	1730	0		A1011	68.696	77.728	27.006		36.75
ATOM	1731	CB		A1011	68.174	77.122	30.588		53.79
ATOM	1732	CG		A1011	67.148	77.215	31.633		53.79
ATOM	1733			A1011	66.008	77.430	31.335		53.79
ATOM	1734	ND2		A1011	67.541	77.071	32.879		53.79
ATOM	1738	N		A1012	69.810	76.638	28.685		25.53
ATOM	1739	CA		A1012	71.016	76.422	27.940		25.53
ATOM	1740	C		A1012	70.747	75.476	26.776	1.00	25.53
ATOM	1741	0		A1012	71.392	75.570	25.756	1.00	25.53
ATOM	1742	CB		A1012	72.118	75.898	28.872	1.00	38.16
ATOM	1743	CG		A1012	71.934	76.312	30.315		38.16
ATOM	1744	CD1		A1012	72.332	75.491	31.341	1.00	38.16
ATOM	1745	CD2		A1012	71.301	77.512	30.645	1.00	38.16
ATOM	1746	CE1		A1012	72.105	75.841	32.642	1.00	38.16
ATOM	1747	CE2		A1012	71.072	77.863	31.943	1.00	38.16
ATOM	1748	CZ		A1012	71.473	77.028	32.927	1.00	38.16
ATOM	1749	OH		A1012	71.240	77.363	34.217	1.00	38.16
ATOM	1752	N		A1013	69.812	74.566	26.863	1.00	71.42
ATOM	1753	CA		A1013	69.638	73.752	25.672	1.00	
MOTA	1754	C	SER	A1013	70.875	72.864	25.398	1.00	71.42

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Inventors: Nancy J. Bump et al.

ATOM	1755	0	SE	R A1013	71.;	360	72.693	24.272	1 00	71.42
ATOM	1756	CB	SE	R A1013	69.3		74.696	24.502	1.00	
ATOM	1757	OG		R A1013	70.4		75.126	23.819	1.00	
MOTA	1760	N	VAI	A1014	71.3		72.310	26.482	1.00	
ATOM	1761	CA.	VAI	A1014	72.5		71.433	26.395		66.71
ATOM	1762	C		A1014	71.9		70.215	26.353	1.00	
ATOM	1763	0		A1014	71.2		70.283	27.994		
ATOM	1764	CB		A1014	73.1		71.888	27.263		66.71
ATOM	1765	CGI		A1014	74.2		73.271	26.795		53.96
ATOM	1766	CG2		A1014	73.4		71.814			53.96
ATOM	1768	N		A1015	72.0		9.104	28.765 26.273		53.96
ATOM	1769	CA		A1015	71.5		57.861	26.273		65.68
ATOM	1770	C		A1015	72.5		6.891			65.68
MOTA	1771	ō		A1015	73.6			27.248		65.68
ATOM	1772	CB		A1015	70.6		6.702	26.646		65.68
ATOM	1773	CG		A1015	69.7		7.214	25.663		100.00
ATOM	1774			A1015			8.179	24.939		100.00
ATOM	1775	CD2		A1015	70.1		8.741	23.734		100.00
ATOM	1776	CEI		A1015	68.5		8.505	25.434		100.00
ATOM	1777	CE2		A1015	69.3		9.596	23.037		100.00
ATOM	1778	CZ			67.6		9.364	24.740		100.00
ATOM	1779	OH		A1015	68.0		9.901	23.546		100.00
ATOM	1782	N			67.2		0.751	22.848		100.00
ATOM	1783	CA		A1016 A1016	72.2		6.269	28.363		55.88
ATOM	1784	C			73.1		5.322	29.008		55.88
ATOM	1785	0		A1016	72.3		4.056	29.380		55.88
ATOM	1786	CB		A1016	71.1		3.996	29.243		55.88
ATOM	1787	OG1		A1016 A1016	73.6		5.988	30.209	1.00	
ATOM	1788	CG2			72.6		5.891	31.280		30.90
ATOM	1791	N N		A1016 A1017	73.8		7.440	29.876		30.90
ATOM	1792	CA		A1017	73.0		3.037	29.840	1.00	99.25
ATOM	1793	C		A1017	72.3		1.822	30.213	1.00	99.25
ATOM	1794	0		A1017	71.8		2.074	31.618	1.00	99.25
ATOM	1795	CB		A1017	72.1		1.294	32.534	1.00	99.25
ATOM	1796	OG1		A1017	73.3		0.593	30.094	1.00	32.66
ATOM	1797	CG2		A1017	72.8		9.789	28.972	1.00	32.66
ATOM	1800	N N		A1017 A1018	73.3		9.770	31.323	1.00	32.66
ATOM	1801	CA		A1018	71.1		3.198	31.786	1.00	18.01
ATOM	1802	C		A1018	70.6		3.569	33.141	1.00	18.01
ATOM	1803	0		A1018	69.3		4.119	32.874	1.00	18.01
ATOM	1804	CB		A1018	68.4		4.021	33.724	1.00	18.01
ATOM	1805	CG		A1018	71.5 71.8		4.623	33.742	1.00	34.98
ATOM	1806	OD1		A1018	71.0		4.337	35.101	1.00	34.98
ATOM	1807	ND2		A1018			4.966	35.982		34.98
ATOM	1811	N		A1018	72.6		3.353	35.331	1.00	
ATOM	1812	CA		A1019			4.679	31.656	1.00	37.97
ATOM	1813	C		A1019	68.2		5.335	30.991		37.97
ATOM	1814	0		A1019	67.8		4.369	29.862	1.00	37.97
ATOM	1815	CB		A1019	67.4		4.733	28.729		37.97
ATOM	1816	OG		A1019	68.7		6.641	30.420	1.00	17.17
ATOM	1819	N		A1019	69.32		6.474	29.138		17.17
ATOM	1820	CA		A1020	67.98		3.097	30.155		31.25
ATOM	1821	CA		A1020 A1020	67.58		2.062	29.225		31.25
ATOM	1822	0		A1020	66.66		1.475	30.328		31.25
ATOM	1823	CB			65.4		1.257	30.127		31.25
ATOM	1824	CG		A1020 A1020	68.7		1.166	28.790		31.83
ATOM	1825			A1020	69.0		1.295	27.302		31.83
	2023	ODI	ASE	M1020	68.28	39 6.	1.870	26.618	T.00	31.83

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Title: Method of Identifying Inhibitors of TIE-2 Inventors: Nancy J. Bump et al.

ATOM 1826 OD2 ASP A1020 70.043 60.869 26.709 1.00 31.83 1828 N VAL A1021 67.214 61.357 31.535 1.00 57.04 ATOM ATOM 1829 CA VAL A1021 66.440 60.813 32.614 1.00 57.04 ATOM 1830 C VAL A1021 65,131 61,522 32,628 1,00 57,04 ATOM 1831 0 VAL A1021 64.091 60.915 32.317 1.00 57.04 MOTA 1832 CB VAL A1021 67.130 60.987 33.916 1.00 94.63 1833 CG1 VAL A1021 ATOM 66.156 60.813 35.032 1.00 94.63 ATOM 1834 CG2 VAL A1021 68.236 59.965 34.012 1.00 94.63 ATOM 1836 N TRP A1022 65.189 62.814 32.960 1.00 51.41 1837 CA TRP A1022 ATOM 64.023 63.696 33.032 1.00 51.41 1838 C TRP A1022 ATOM 63.002 63.457 31.908 1.00 51.41 ATOM 1839 O TRP A1022 61.815 63.252 32.147 1.00 51.41 ATOM 1840 CB TRP A1022 64.519 65.133 33.005 1.00 32.10 1841 CG TRP A1022 ATOM 63.422 66.227 32.925 1.00 32.10 62.602 66.469 31.868 1.00 32.10 ATOM 1842 CD1 TRP A1022 ATOM 1843 CD2 TRP A1022 63.068 67.160 33.938 1.00 32.10 ATOM 1844 NE1 TRP A1022 61.779 67.469 32.157 1.00 32.10 1845 CE2 TRP A1022 61.779 67.469 32.157 1.00 32.10 1846 CE3 TRP A1022 62.032 67.931 33.428 1.00 32.10 1846 CE2 TRP A1022 63.526 67.420 35.221 1.00 32.10 1847 C22 TRP A1022 62.921 68.481 35.978 1.00 32.10 1848 CZ3 TRP A1022 62.921 68.481 35.978 1.00 32.10 1852 N SER A1023 63.472 63.525 30.671 1.00 66.03 1853 CA SER A1023 62.598 63.263 29.546 1.00 66.03 1855 C SER A1023 62.598 63.263 29.546 1.00 66.03 1855 O SER A1023 60.717 61.903 30.036 1.00 66.03 1855 O SER A1023 60.717 61.903 30.036 1.00 66.03 1855 O SER A1023 63.734 64.377 27.752 1.00 96.89 1857 OG SER A1023 62.719 60.909 30.036 1.00 61.41 1861 CA TYR A1024 62.719 60.909 30.106 1.00 11.41 1862 C TYR A1024 62.238 59.645 30.472 1.00 11.41 1862 C TYR A1024 62.821 59.567 30.982 1.00 11.41 1866 CD TYR A1024 62.821 56.581 30.474 1.00 14.38 1866 CD1 TYR A1024 62.821 56.581 30.474 1.00 14.38 1868 CE1 TYR A1024 62.821 56.581 30.474 1.00 14.38 1868 CE1 TYR A1024 62.821 56.581 30.474 1.00 14.38 1869 CE2 TYR A1024 61.765 55.987 30.993 1.00 14.38 1869 CE2 TYR A1024 61.765 55.987 30.993 1.00 14.38 1869 CE2 TYR A1024 61.765 55.987 30.993 1.00 14.38 1869 CE2 TYR A1024 61.765 55.987 30.993 1.00 14.38 1869 CE2 TYR A1024 61.765 55.987 30.993 1.00 14.38 1869 CE2 TYR A1024 61.765 55.987 30.993 1.00 14.38 1870 CZ TYR A1024 61.765 55.987 30.993 1.00 14.38 1870 CZ TYR A1024 61.765 55.987 30.993 1.00 14.38 1870 CZ TYR A1024 61.765 55.987 30.993 1.00 14.38 1870 CZ TYR A1024 61.765 55.987 30.993 1.00 14.38 1870 CZ TYR A1024 61.765 55.987 30.993 1.00 14.38 1870 CZ TYR A1024 61.765 55.987 30.993 1.00 14.38 1871 OR TYR A1024 61.765 55.987 30.993 1.00 14.38 1875 CZ TYR A1024 61.765 55.987 30.993 1.00 14.38 1875 CZ CY TYR A1024 61.765 55.987 30.993 1.00 14.38 1875 CZ CY TYR A1024 61.765 55.987 30.993 1.00 14.38 1875 CZ CY TYR A1024 61.765 55.987 30.2073 1.00 14.38 1875 CZ CY TYR A1024 61.765 55.987 30.2073 1.00 14.38 1875 CZ CY TYR A1024 61.765 55.987 30.2073 1.00 14.38 1875 CZ CY TYR A1024 61.765 55.987 30.2073 1.00 14.38 1875 CZ CY TYR A1024 61.765 55.987 30.2073 1.00 14.38 1875 CZ CY TY ATOM 1845 CE2 TRP A1022 62.032 67.931 33.428 1.00 32.10 MOTA MOTA ATOM MOTA ATOM ATOM ATOM MOTA ATOM ATOM MOTA ATOM MOTA 1874 N GLY A1025 1875 CA GLY A1025 MOTA 59.678 60.385 33.207 1.00 29.83 58.509 61.033 32.430 1.00 29.83 1876 C GLY A1025 MOTA ATOM 1877 O GLY A1025 57.356 60.716 32.652 1.00 29.83 ATOM 1879 N VAL A1026 58.762 61.985 31.554 1.00 67.56 ATOM 1880 CA VAL A1026 57.615 62.466 30.859 1.00 67.56 ATOM 1881 C VAL A1026 57.199 61.121 30.271 1.00 67.56 MOTA 1882 O VAL A1026 56.204 60.589 30.705 1.00 67.56 1883 CB VAL A1026 ATOM 57.975 63.548 29.836 1.00 59.88 MOTA 1884 CG1 VAL A1026 56.872 64.579 29.759 1.00 59.88 1885 CG2 VAL A1026 ATOM 59.232 64.199 30.249 1.00 59.88 MOTA 1887 N LEU A1027 57.982 60.546 29.354 1.00 31.95 ATOM 1888 CA LEU A1027 57.703 59.178 28.787 1.00 31.95 ATOM 1889 C LEU A1027 57.056 58.236 29.865 1.00 31.95 1890 O LEU A1027 ATOM 55.988 57.621 29.691 1.00 31.95 59.000 58.502 28.304 1.00 37.14 1891 CB LEU A1027 MOTA 1892 CG LEU A1027 MOTA 58.894 57.447 27.219 1.00 37.14

ATOM	1893			J A1027	57.496	57.117	27.007	1.00 37.14
ATOM	1894	CD2		A1027	59.417	57.890	25.930	1.00 37.14
ATOM	1896	N	LEU	A1028	57.746	58.125	30.978	1.00 8.77
ATOM	1897	CA		J A1028	57.188	57.363	32.009	1.00 8.77
ATOM	1898	C	LEU	A1028	55.743	57.749	32.088	1.00 8.77
ATOM	1899	0	LEU	A1028	54.947	56.870	31.744	1.00 8.77
ATOM	1900	CB	LEU	A1028	57.875	57.508	33.363	1.00 48.45
ATOM	1901	CG	LEU	A1028	57.252	56.440	34.294	1.00 48.45
ATOM	1902	CD1	LEU	A1028	56.823	55.185	33.534	1.00 48.45
ATOM	1903	CD2	LEU	A1028	58.220	56.043	35.333	1.00 48.45
ATOM	1905	N		A1029	55.442	59.029	32.483	1.00 30.07
ATOM	1906	CA	TRP		54.084	59.703	32.660	1.00 30.07
ATOM	1907	C	TRP		53.253	59.613	31.429	1.00 30.07
ATOM	1908	ō		A1029	52.118	59.261	31.397	1.00 30.07
ATOM	1909	CB		A1029	54.227	61.222	32.983	
ATOM	1910	CG	TRP		52.932	62.000	33.312	1.00 2.92
ATOM	1911	CD1		A1029	52.349	62.276	34.582	1.00 2.92
ATOM	1912	CD2		A1029	51.964			1.00 2.92
ATOM	1913	NE1	TRP			62.434	32.334	1.00 2.92
ATOM	1914	CE2		A1029	51.050	62.846	34.369	1.00 2.92
ATOM	1915	CE3		A1029	50.827	62.919	33.011	1.00 2.92
ATOM	1916	CZ2			51.955	62.444	30.937	1.00 2.92
ATOM	1917			A1029	49.767	63.362	32.342	1.00 2.92
		CZ3	TRP		50.836	62.910	30.283	1.00 2.92
ATOM	1918	CH2		A1029	49.791	63.345	30.971	1.00 2.92
ATOM	1921	N		A1030	53.881	60.008	30.382	1.00 26.20
ATOM	1922	CA		A1030	53.292	59.957	29.076	1.00 26.20
ATOM	1923	C		A1030	52.824	58.589	28.725	1.00 26.20
ATOM	1924	0		A1030	52.344	58.417	27.638	1.00 26.20
ATOM	1925	CB		A1030	54.358	60.378	28.077	1.00 24.00
ATOM	1926	CG		A1030	53.879	60.996	26.869	1.00 24.00
ATOM	1927	CD		A1030	54.860	60.718	25.857	1.00 24.00
ATOM	1928	OEl		A1030	55.885	60.279	26.378	1.00 24.00
ATOM	1929	OE2		A1030	54.661	60.907	24.633	1.00 24.00
MOTA	1931	N		A1031	52.969	57.631	29.631	1.00 14.69
ATOM	1932	CA.		A1031	52.633	56.216	29.376	1.00 14.69
ATOM	1933	C	ILE	A1031	51.704	55.738	30.426	1.00 14.69
ATOM	1934	0	ILE	A1031	51.033	54.761	30.203	1.00 14.69
MOTA	1935	CB	ILE	A1031	53.923	55.272	29.416	1.00 33.44
ATOM	1936	CG1	ILE	A1031	54.294	54.757	28.021	1.00 33.44
ATOM	1937	CG2	ILE	A1031	53.671	53.993	30.253	1.00 33.44
ATOM	1938	CD1	ILE	A1031	55.762	54.225	27.948	1.00 33.44
ATOM	1940	N	VAL	A1032	51.726	56.285	31.621	1.00 14.19
MOTA	1941	CA	VAL	A1032	50.676	55.868	32.559	1.00 14.19
MOTA	1942	C	VAL	A1032	49.327	56.496	32.011	1.00 14.19
ATOM	1943	0	VAL	A1032	48.282	55.823	31.882	1.00 14.19
ATOM	1944	CB		A1032	50.924	56.349	33.944	1.00 41.51
ATOM	1945	CG1		A1032	49.666	56.640	34.596	1.00 41.51
ATOM	1946	CG2		A1032	51.581	55.290	34.704	1.00 41.51
ATOM	1948	N		A1033	49.395	57.755	31.625	1.00 31.81
MOTA	1949	CA		A1033	48.320	58.505	31.065	1.00 31.81
ATOM	1950	C		A1033	47.658	57.730	29.910	
ATOM	1951	Ö		A1033	46.551	58.079	29.910	
ATOM	1952	CB		A1033	48.895	59.828		1.00 31.81
ATOM	1953	OG		A1033	49.757		30.546	1.00 68.54
ATOM	1956	N		A1033	48.316	59.623	29.445	1.00 68.54
ATOM	1957	CA		A1034 A1034		56.686	29.442	1.00 2.00
ATOM	1958	C			47.777	55.984	28.298	1.00 2.00
ATOM	1220	-	ಸಚಿ	A1034	47.645	56.833	26.999	1.00 2.00

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Nancy J. Bump et al.

Inventors:

46.584 56.955 26.409 1.00 2.00 ATOM 1959 O LEU A1034 1960 CB LEU A1034 46.422 55.343 28.654 1.00 31.43 ATOM ATOM 1961 CG LEU A1034 46.478 53.883 29.207 1.00 31.43 ATOM 1962 CD1 LEU A1034 45.072 53.333 29.484 1.00 31.43 MOTA 1963 CD2 LEU A1034 47.244 52.988 28.207 1.00 31.43 48.706 57.372 26.438 1.00 4.53 ATOM 1965 N GLY A1035 1966 CA GLY A1035 48.437 58.149 25.224 1.00 4.53 ATOM 48.241 59.685 25.565 1.00 4.53 MOTA 1967 C GLY A1035 ATOM 1968 0 GLY A1035 47.964 60.498 24.649 1.00 4.53
ATOM 1970 N GLY A1036 48.509 60.071 26.820 1.00 18.31
ATOM 1971 CA GLY A1036 48.281 61.470 27.160 1.00 18.31
ATOM 1972 C GLY A1036 49.211 62.717 27.185 1.00 18.31
ATOM 1973 O GLY A1036 49.988 62.881 28.181 1.00 18.31
ATOM 1973 N THR A1037 49.027 63.591 26.164 1.00 48.85
ATOM 1976 CA THR A1037 49.027 63.591 26.164 1.00 48.85
ATOM 1977 C THR A1037 49.027 63.591 26.164 1.00 48.85
ATOM 1978 O THR A1037 49.431 65.933 28.077 1.00 48.85
ATOM 1979 CB THR A1037 48.988 65.984 25.216 1.00 25.15
ATOM 1980 OGI THR A1037 48.988 65.994 23.772 1.00 25.15
ATOM 1981 CQ2 THR A1037 48.988 65.904 23.772 1.00 25.15
ATOM 1986 C PRO A1038 51.538 65.697 27.456 1.00 42.23
ATOM 1986 C PRO A1038 51.538 65.697 27.456 1.00 42.23
ATOM 1986 C PRO A1038 51.496 66.239 28.775 1.00 42.23
ATOM 1986 C PRO A1038 51.496 67.691 28.995 1.00 42.23
ATOM 1989 CG PRO A1038 53.271 65.779 99.048 1.00 10.66
ATOM 1991 N TYR A1039 51.381 68.090 30.253 1.00 39.67
ATOM 1993 C TYR A1037 49.924 69.987 29.622 1.00 39.67
ATOM 1994 O TYR A1039 51.381 68.090 30.253 1.00 39.67
ATOM 1995 CG TYR A1039 51.381 68.090 30.253 1.00 39.67
ATOM 1995 CG TYR A1039 51.381 68.090 30.553 1.00 39.67
ATOM 1996 CG TYR A1039 51.381 68.090 30.553 1.00 39.67
ATOM 1997 CTYR A1039 51.366 69.951 30.3756 1.00 39.67
ATOM 1999 CTYR A1039 52.566 70.457 30.3755 1.00 39.67
ATOM 1995 CG TYR A1039 52.566 70.457 30.3755 1.00 39.67
ATOM 1995 CG TYR A1039 53.503 69.958 31.103 1.00 15.36
ATOM 1995 CG TYR A1039 53.503 69.958 31.103 1.00 15.36
ATOM 1995 CG TYR A1039 53.503 69.958 31.103 1.00 15.36
ATOM 1995 CG TYR A1039 53.503 69.958 31.103 1.00 15.36
ATOM 1996 CG TYR A1039 53.503 69.958 31.103 1.00 15.36
ATOM 1997 CD TYR A1039 54.636 69.951 32.481 1.00 15.36
ATOM 1998 CG TYR A1039 55.730 69.157 31.105 1.00 15.36
ATOM 2000 CG2 TYR A1039 55.737 69.191 32.449 1.00 15.36
ATOM 2001 CZ TYR A1039 55.737 69.191 32.449 1.00 15.36
ATOM 2007 C CYS A1040 47.597 69.681 28.882 1.00100.00
ATOM 2008 O CYS A1040 47.597 69.681 28.882 1.00100.00 1968 O GLY A1035 47.964 60.498 24.649 1.00 4.53 ATOM 1970 N GLY A1036 48.509 60.071 26.820 1.00 18.31 ATOM ATOM 2008 O CYS A1040 46.711 70.987 30.625 1.00100.00 ATOM 2009 CB CYS A1040 46.507 68.566 28.832 1.00 63.76 ATOM 2010 SG CYS A1040 45.039 68.722 27.619 1.00 63.76 ATOM 2012 N GLY A1041 46.836 71.938 28.605 1.00 75.53 MOTA 2013 CA GLY A1041 46.305 73.175 29.127 1.00 75.53 2014 C GLY A1041 47.419 74.160 29.448 1.00 75.53 ATOM 2015 O GLY A1041 47.217 75.358 29.342 1.00 75.53 ATOM 48.581 73.668 29.868 1.00 27.54 2017 N MET A1042 ATOM 2017 N MET Al042 48.581 73.668 29.868 1.00 27.54
2018 CA MET Al042 49.666 74.553 30.126 1.00 27.54
2019 C MET Al042 50.119 75.065 28.731 1.00 27.54
2020 O MET Al042 50.034 74.344 27.742 1.00 27.54
2021 CB MET Al042 50.034 74.346 32.298 1.00 47.82
2022 CG MET Al042 51.032 74.460 32.298 1.00 47.82
2023 SD MET Al042 52.810 74.502 32.805 1.00 47.82
2024 CE MET Al042 52.729 74.790 34.564 1.00 47.82 ATOM ATOM ATOM ATOM ATOM MOTA ATOM

Docket/App No.: 2079.1037-001

Title: Method of Identifying Inhibitors of TIE-2 Inventors: Nancy J. Bump et al.

ATOM	2026	N	THR	A1043	50.481	76.351	28.681	1 00	59.25
ATOM	2027	CA		A1043	50.918	77.067	27.468		59.25
ATOM	2028	C		A1043	52.434	76.937	27.397		59.25
ATOM	2029	0		A1043	53.084				
ATOM	2030	CB		A1043	50.586	76.835	28.437		59.25
ATOM	2030	OG1		A1043		78.617	27.528		62.50
ATOM	2031	CG2			51.070	79.181	28.773		62.50
ATOM	2032			A1043	49.076	78.877	27.351		62.50
		N		A1044	52.997	76.968	26.194		100.00
ATOM	2036	CA		A1044	54.435	76.799	26.060		100.00
ATOM	2037	C		A1044	55.282	77.679	26.975		100.00
ATOM	2038	0		A1044	56.478	77.467	27.100		100.00
ATOM	2039	CB		A1044	54.857	76.963	24.601	1.00	77.67
ATOM	2040	SG		A1044	54.890	75.383	23.687	1.00	77.67
ATOM	2042	N		A1045	54.673	78.663	27.623	1.00	100.00
ATOM	2043	CA		A1045	55.425	79.501	28.548	1.001	100.00
ATOM	2044	C		A1045	54.810	79.446	29.910	1.001	100.00
ATOM	2045	0		A1045	55.455	79.833	30.878	1.001	100.00
MOTA	2046	CB	ALA	A1045	55.461	80.899	28.107	1.00	35.04
MOTA	2048	N	GLU	A1046	53.550	79.023	30.018	1.00	27.64
ATOM	2049	CA		A1046	53.057	78.932	31.346	1.00	27.64
MOTA	2050	C	GLU	A1046	54.177	78.018	31.917	1.00	27.64
ATOM	2051	0	GLU	A1046	54.507	78.117	33.092	1.00	27.64
ATOM	2052	CB	GLU	A1046	51.665	78.264	31.365	1.00	79.70
ATOM	2053	CG	GLU	A1046	50.465	79.239	31.521	1.00	79.70
MOTA	2054	CD	GLU	A1046	49.180	78.818	30.745	1.00	79.70
ATOM	2055	OE1	GLU	A1046	48.058	79.216	31.128	1.00	79.70
ATOM	2056	OE2		A1046	49.264	78.096	29.748		79.70
MOTA	2058	N	LEU	A1047	54.800	77.199	31.050	1.00	83.80
ATOM	2059	CA	LEU	A1047	55.871	76.230	31.413	1.00	83.80
MOTA	2060	C	LEU	A1047	57.286	76.737	31.646	1.00	83.80
ATOM	2061	0	LEU	A1047	57.838	76.529	32.712		83.80
MOTA	2062	CB	LEU	A1047	55.968	75.119	30.368	1.00	39.62
ATOM	2063	CG	LEU	A1047	55.167	73.857	30.626		39.62
ATOM	2064	CD1	LEU	A1047	55.186	73.119	29.339		39.62
ATOM	2065	CD2	LEU	A1047	55.697	73.034	31.803	1.00	39.62
ATOM	2067	N	TYR	A1048	57.904	77.315	30.615		32.07
MOTA	2068	CA	TYR	A1048	59.235	77.894	30.746		32.07
ATOM	2069	C	TYR	A1048	59.043	78.647	32.109		32.07
ATOM	2070	0	TYR	A1048	59.704	78.383	33.115		32.07
ATOM	2071	CB	TYR	A1048	59.498	78.877	29.566	1.00	14.15
ATOM	2072	CG	TYR	A1048	60.160	78.333	28.256		14.15
ATOM	2073	CD1	TYR	A1048	59.401	77.982	27.165		14.15
ATOM	2074	CD2	TYR	A1048	61.563	78.249	28.095		14.15
ATOM	2075	CE1	TYR	A1048	59.969	77.565	25.934		14.15
ATOM	2076	CE2	TYR	A1048	62.137	77.841	26.871		14.15
ATOM	2077	CZ		A1048	61.359	77.502	25.784		14.15
MOTA	2078	OH	TYR	A1048	61.927	77.135	24.513		14.15
MOTA	2081	N	GLU	A1049	58.055	79.533	32.169		36.64
MOTA	2082	CA	GLU	A1049	57.811	80.267	33.390		36.64
ATOM	2083	C		A1049	57.770	79.384	34.578	1.00	
ATOM	2084	0		A1049	58.757	79.290	35.320	1.00	
ATOM	2085	CB		A1049	56.500	81.002	33.368	1.00	
ATOM	2086	CG		A1049	56.151	81.544	34.760		35.78
ATOM	2087	CD		A1049	54.683	81.875	34.899		35.78
ATOM	2088	OE1		A1049	53.989	82.043	33.858	1.00	
ATOM	2089	OE2		A1049	54.252	81.947	36.060		35.78
ATOM	2091	N		71050	56 601	70 777	34.700	1.00	00.70

FIG. 6DD ,~

56.601 78.737 34.708 1.00 93.85

ATOM 2091 N LYS A1050

ATOM	2092	CA	LYS	A1050	56.197	77.839	35.793	1.00 93.85
ATOM	2093	C	LYS	A1050	57.046	76.622	36.085	1.00 93.85
ATOM	2094	0	LYS	A1050	57.178	76.212	37.231	1.00 93.85
ATOM	2095	CB		A1050	54.752	77.418	35.584	1.00 86.89
ATOM	2097	N		A1051	57.599	76.008	35.063	1.00 40.78
ATOM	2098	CA		A1051	58.458	74.868	35.336	1.00 40.78
ATOM	2099	C		A1051	59.412	75.166	36.508	1.00 40.78
								1.00 40.78
ATOM	2100	0		A1051	59.321	74.483	37.539	
ATOM	2101	CB		A1051	59.201	74.391	34.072	1.00 66.80
ATOM	2102	CG		A1051	58.984	72.898	33.726	1.00 66.80
ATOM	2103	CD1		A1051	57.754	72.376	34.370	1.00 66.80
ATOM	2104	CD2		A1051	58.875	72.719	32.253	1.00 66.80
ATOM	2106	N		A1052	60.356	76.129	36.369	1.00 42.79
ATOM	2107	CA		A1052	61.299	76.504	37.431	1.00 42.79
MOTA	2108	C		A1052	60.655	76.803	38.741	1.00 42.79
ATOM	2109	0	PRO	A1052	61.311	76.783	39.783	1.00 42.79
ATOM	2110	CB	PRO	A1052	61.928	77.731	36.906	1.00 29.07
ATOM	2111	CG	PRO	A1052	61.952	77.549	35.473	1.00 29.07
ATOM	2112	CD	PRO	A1052	60.713	76.805	35.110	1.00 29.07
ATOM	2113	N	GLN	A1053	59.365	77.114	38.699	1.00 68.39
ATOM	2114	CA		A1053	58.662	77.426	39.921	1.00 68.39
ATOM	2115	C		A1053	58.823	76.206	40.781	1.00 68.39
ATOM	2116	0		A1053	58.934	76.303	41.999	1.00 68.39
ATOM	2117	CB		A1053	57.200	77.701	39.646	1.00100.00
ATOM	2119	N		A1054	58.852	75.049	40.125	1.00 93.49
ATOM	2120	CA		A1054	59.012	73.776	40.808	1.00 93.49
ATOM	2121	C		A1054	57.849	72.863	40.494	1.00 93.49
ATOM	2122	ō		A1054	57.727	71.794	41.065	1.00 93.49
ATOM	2124	N		A1055	57.000	73.311	39.577	1.00 23.98
		CA						
ATOM	2125			A1055	55.804	72.609	39.141	1.00 23.98
ATOM	2126	C		A1055	56.207	71.481	38.197	1.00 23.98
ATOM	2127	0_		A1055	57.062	71.702	37.321	1.00 23.98
ATOM	2128	CB		A1055	54.869	73.579	38.415	1.00 76.79
ATOM	2129	CG		A1055	53.703	72.894	37.769	1.00 76.79
MOTA	2130	CD1		A1055	52.547	72.645	38.480	1.00 76.79
ATOM	2131	CD2		A1055	53.803	72.391	36.479	1.00 76.79
MOTA	2132	CE1		A1055	51.516	71.891	37.927	1.00 76.79
ATOM	2133	CE2	TYR	A1055	52.788	71.639	35.913	1.00 76.79
ATOM	2134	CZ	TYR	A1055	51.647	71.382	36.644	1.00 76.79
ATOM	2135	OH	TYR	A1055	50.677	70.559	36.119	1.00 76.79
ATOM	2138	N	ARG	A1056	55.598	70.299	38.398	1.00 28.98
ATOM	2139	CA	ARG	A1056	55.835	69.092	37.633	1.00 28.98
ATOM	2140	C	ARG	A1056	54.472	68.506	37.281	1.00 28.98
ATOM	2141	0	ARG	A1056	53.443	68.997	37.844	1.00 28.98
ATOM	2142	CB	ARG	A1056	56.540	68.057	38.504	1.00 43.74
ATOM	2143	CG	ARG	A1056	57.930	68.420	39.046	1.00 43.74
ATOM	2144	CD	ARG	A1056	58.890	68.928	37.990	1.00 43.74
ATOM	2145	NE		A1056	59.420	70.184	38.476	1.00 43.74
ATOM	2146	CZ		A1056	60.710	70.421	38.632	1.00 43.74
ATOM	2147	NH1		A1056	61.589	69.481	38.326	1.00 43.74
ATOM	2148	NH2		A1056	61.113	71.570	39.153	1.00 43.74
ATOM	2155	N		A1057	54.457	67.425	36.423	1.00 3.74
ATOM	2156	CA		A1057	53.199	66.719	36.037	1.00 3.73
ATOM	2157	C		A1057		66.273	37.247	1.00 3.73
ATOM	2157	0		A1057 A1057	52.455		37.247	1.00 3.73
ATOM					53.013	65.940		
	2159	CB		A1057	53.453	65.540	35.129	1.00 53.30
ATOM	2160	CG	TIRO	A1057	53.594	65.965	33.659	1.00 53.30

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ATOM	2161	CD1	LEU	A1057	54.129	64.770	32.869	1.00 53.30
ATOM	2162			A1057	52.271	66.541	33.071	1.00 53.30
ATOM	2164	N		A1058	51.138	66.322	37.070	1.00 13.17
ATOM	2165	CA		A1058	50.076	65.947	38.013	1.00 13.17
ATOM	2166	C		A1058	50.122	64.399	38.274	1.00 13.17
ATOM	2167	0		A1058	50.140	63.602	37.310	1.00 13.17
ATOM	2168	CB		A1058	48,779	66.341	37.327	1.00 48.21
ATOM	2169	CG		A1058	48.686	65.807	35.864	1.00 48.21
ATOM	2170	CD		A1058	49.433	66.661	34.827	1.00 48.21
ATOM	2171	OE1	GLU	A1058	50.080	67.619	35.269	1.00 48.21
ATOM	2172	OE2	GLU	A1058	49.379	66.410	33.589	1.00 48.21
ATOM	2174	N	LYS	A1059	50.163	63.947	39.531	1.00 35.98
ATOM	2175	CA	LYS	A1059	50.196	62.496	39.689	1.00 35.98
ATOM	2176	C	LYS	A1059	49.010	62.039	38.876	1.00 35.98
ATOM	2177	0	LYS	A1059	47.980	62.696	38.847	1.00 35.98
ATOM	2178	CB	LYS	A1059	50.046	62.040	41.118	1.00 48.90
ATOM	2179	CG	LYS	A1059	50.101	60.540	41.194	1.00 48.90
ATOM	2180	CD	LYS	A1059	50.190	60.048	42.616	1.00 48.90
ATOM	2181	CE	LYS	A1059	48.873	59.367	43.057	1.00 48.90
ATOM	2182	NZ	LYS	A1059	48.940	57.857	43.104	1.00 48.90
ATOM	2187	N	PRO	A1060	49.129	60.936	38.161	1.00 50.25
ATOM	2188	CA	PRO	A1060	47.931	60.601	37.405	1.00 50.25
ATOM	2189	C	PRO	A1060	46.928	59.608	37.964	1.00 50.25
MOTA	2190	0	PRO	A1060	47.176	58.424	37.967	1.00 50.25
ATOM	2191	CB	PRO	A1060	48.504	60.174	36.084	1.00 21.32
ATOM	2192	CG	PRO	A1060	50.037	59.963	36.356	1.00 21.32
ATOM	2193	CD	PRO	A1060	50.246	60.058	37.817	1.00 21.32
ATOM	2194	N		A1061	45.772	60.120	38.395	1.00 35.93
ATOM	2195	CA		A1061	44.633	59.371	38.985	1.00 35.93
MOTA	2196	C	LEU	A1061	44.746	57.870	39.239	1.00 35.93
MOTA	2197	0		A1061	44.731	57.415	40.396	1.00 35.93
MOTA	2198	CB		A1061	43.368	59.617	38.155	1.00 74.38
MOTA	2199	CG		A1061	43.355	59.574	36.617	1.00 74.38
MOTA	2200			A1061	44.689	59.971	35.997	1.00 74.38
ATOM	2201	CD2		A1061	42.942	58.174	36.185	1.00 74.38
ATOM	2203	M		A1062	44.864	57.145	38.117	1.00 56.10
ATOM	2204	CA		A1062	44.988	55.689	37.947	1.00 56.10
ATOM	2205	C		A1062	46.399	55.281	38.291	1.00 56.10
ATOM	2206	0		A1062	46.855	54.240	37.822	1.00 56.10
ATOM	2207	CB		A1062	44.865	55.366	36.477	
ATOM	2208	CG		A1062	46.002	56.035	35.686	1.00 38.56
ATOM	2209	OD1		A1062	46.683	56.890	36.256	1.00 38.56
ATOM	2210	ND2		A1062	46.216	55.673 56.092	34.397 39.065	1.00 38.36
ATOM	2214	N		A1063	47.109			1.00 99.97
ATOM	2215	CA		A1063	48.503	55.791	39.376 40.829	1.00 99.97
ATOM	2216	C		A1063	48.861	55.613 56.299	41.699	1.00 99.97
ATOM	2217	0		A1063	48.362	56.299	38.827	1.00 81.22
ATOM	2218	CB		A1063	49.398		37.527	1.00 81.22
ATOM	2219	SG		A1063 A1064	50.449 49.770	56.431 54.691	41.070	1.00 81.22
ATOM	2221	N		A1064	49.770 50.260	54.691	42.405	1.00 40.11
ATOM	2222	CA C		A1064	51.472	55.243	42.405	1.00 40.11
ATOM ATOM	2223	0		A1064	51.4/2	55.243	42.013	1.00 40.11
ATOM	2224	CB		A1064	50.623	52.961	42.560	1.00 40.11
ATOM	2225	CG		A1064	50.760	52.580	43.992	1.00 60.57
ATOM	2227			A1064	50.671	53.492	44.844	1.00 60.57
ATOM	2228	OD2		A1064	50.941	51.391	44.292	1.00 60.57
WI OIL	2220	002	2.00		30.341	22.022		

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Title: Method of Identifying Inhibitors of TIE-2 Inventors: Nancy J. Bump et al.

MOTA	2230	N	ASP	A1065	5	1.409	55.	855	43.980	1.00	46.39
ATOM	2231	CA	ASP	A1065		2.499	56.		44.508		46.39
ATOM	2232	C	ASP	A1065	5	3.984	56.	043	44.229		46.39
ATOM	2233	0	ASP	A1065		4.869	56.		44.124		46.39
ATOM	2234	CB	ASP	A1065	52	2.299	56.1		46.02	1.00	75.00
ATOM	2235	CG		A1065		1.156	57.1		46.357		75.00
ATOM	2236	OD1		A1065		0.426	58.		45.452		75.00
MOTA	2237	OD2		A1065		0.988	58.		47.550		75.00
ATOM	2239	N		A1066		3.951	54.		44.107		29.06
MOTA	2240	CA		A1066		5.205	54.		43.803		29.06
ATOM	2241	C		A1066		5.543	54.		42.403		29.06
ATOM	2242	0	GLU	A1066		5.559	55.		42.220		29.06
ATOM	2243	CB		A1066		5.109	52.		43.888		46.46
MOTA	2244	CG	GLU	A1066		5.488	51.1		43.899		46.46
ATOM	2245	CD		A1066		5.612	50.6		44.880		46.46
MOTA	2246	OE1		A1066		5.711	50.5		45.759		46.46
ATOM	2247	OE2		A1066		7.616	49.5		44.765		46.46
ATOM	2249	N		A1067		1.727	54.		41.416		32.03
ATOM	2250	CA		A1067		5.023	54.5		40.036		
ATOM	2251	C		A1067		5.293	56.6		39.733		
ATOM	2252	ō		A1067		5.029	56.4		38.812		32.03
ATOM	2253	CB		A1067		3.885	54.0		39.107		15.97
ATOM	2254	CG1		A1067		3.965	54.6		37.618		15.97
ATOM	2255	CG2		A1067		3.929	52.4		39.087		15.97
ATOM	2257	N		A1068		1.738	56.9		40.480		40.19
ATOM	2258	CA		A1068		5.001	58.3		40.091		40.19
ATOM	2259	C		A1068		5.057	58.9		40.941		40.19
ATOM	2260	0		A1068		5.899	59.		40.422		
ATOM	2261	CB		A1068		3.684	59.0		40.422		
ATOM	2262	CG		A1068		3.658	60.5		40.344		3.92
ATOM	2263	CD1		A1068		3.484	61.3		39.326		
ATOM	2264	CD2		A1068		3.650	60.9		41.607		
ATOM	2265	CE1		A1068		3.296	62.		39.530		
ATOM	2266	CE2		A1068		3.473	62.2		41.862		
ATOM	2267	CZ		A1068		3.311	63.1		40.812		
ATOM	2268	OH		A1068		3.384	64.5		41.015		3.92
ATOM	2271	N		A1069		5.999	58.		42.242		
ATOM	2272	CA		A1069		7.036	59.2		43.139		
ATOM	2272	CA		A1069		3.139	58.2		42.723		
ATOM	2274	Ö		A1069		3.415	57.3		43.454		
ATOM	2275	CB		A1069		5.639	58.5		44.588		80.97
ATOM	2276	CG		A1069		7.819	58.9		45.514		80.97
ATOM	2277	OD1		A1069		9.968	59.0		45.061		80.97
ATOM	2278	OD2		A1069		7.591			46.714		80.97
ATOM	2270	N N					58.				
ATOM	2280	CA		A1070 A1070		3.667	58.5		41.503		
ATOM	2281	CA		A1070		9.682	57.8		40.729		
						9.701	58.		39.408		
ATOM	2283	0		A1070		0.763	58.1		38.932		
ATOM	2284	CB		A1070		9.389	56.3		40.348		35.45
ATOM	2285	CG		A1070		0.432	56.1		39.208		35.45
MOTA	2286	CD1		A1070		1.722	55.		39.890		
MOTA	2287	CD2		A1070		0.081	54.		38.223		35.45
MOTA	2289	N		A1071		8.577	58.		38.714		33.43
ATOM	2290	CA		A1071		B.662	59.		37.490		33.43
ATOM	2291	C		A1071		9.072	60.		37.999		
ATOM	2292	0		A1071		9.717	61.		37.30		
ATOM	2293	CB	MET	A1071	5	7.328	59.	425	36.71	b 1.00	46.26

ATOM	2294	CG	MET	A1071	56.293	60.425	37.126	1.00	46.26
ATOM	2295	SD	MET	A1071	54.669	59.634	37.210		46.26
ATOM	2296	CE		A1071	54.450	58.978	35.595	1.00	
ATOM	2298	N		A1072	58.729	61.126	39.238	1.00	
ATOM	2299	CA		A1072	59.114	62.389	39.800	1.00	
ATOM	2300	C		A1072	60.612	62.482	40.123	1.00	
ATOM	2301	ō		A1072	61.232	63.557			
ATOM	2302	CB		A1072	58.293	62.660	40.039		27.25
ATOM	2303	CG		A1072			41.064		100.00
ATOM	2304	CD		A1072	56.890	63.206	40.805		100.00
ATOM	2305	NE		A1072	56.900	64.723	40.605		100.00
ATOM	2305	CZ			57.085	65.438	41.861		100.00
ATOM	2306			A1072	56.517	66.600	42.150		100.00
		NH1		A1072	55.722	67.184	41.271		100.00
ATOM	2308	NH2		A1072	56.749	67.178	43.315		100.00
ATOM	2315	N		A1073	61.212	61.376	40.533		63.04
ATOM	2316	CA		A1073	62.625	61.439	40.836	1.00	63.04
ATOM	2317	C		A1073	63.329	61.922	39.571	1.00	63.04
ATOM	2318	0		A1073	64.270	62.702	39.623	1.00	63.04
ATOM	2319	CB	GLN	A1073	63.152	60.060	41.233	1.00	85.05
ATOM	2320	CG		A1073	62.417	59.384	42.387	1.00	85.05
MOTA	2321	CD	GLN	A1073	63.134	58.127	42.896	1.00	85.05
MOTA	2322	OE1	GLN	A1073	62.615	57.410	43.752	1.00	85.05
ATOM	2323	NE2	GLN	A1073	64.322	57.859	42.364		85.05
ATOM	2327	N	CYS	A1074	62.838	61.488	38.421		37.06
ATOM	2328	CA	CYS	A1074	63.456	61.841	37.163		37.06
ATOM	2329	C	CYS	A1074	63.305	63.280	36.845		37.06
MOTA	2330	0	CYS	A1074	63.613	63.703	35.747		37.06
ATOM	2331	CB	CYS	A1074	62.838	61.039	36.021		55.92
MOTA	2332	SG	CYS	A1074	62.574	59.373	36.414		55.92
MOTA	2334	N	TRP	A1075	62.780	64.030	37.793	1.00	54.40
ATOM	2335	CA	TRP	A1075	62.549	65.443	37.559		54.40
ATOM	2336	С	TRP	A1075	63.051	66.360	38.693		54.40
MOTA	2337	0	TRP	A1075	62.683	67.533	38.757		54.40
ATOM	2338	CB	TRP	A1075	61.055	65.719	37.347		13.83
ATOM	2339	CG	TRP	A1075	60.306	65.009	36.268		13.83
ATOM	2340	CD1	TRP	A1075	60.694	64.793	34.985	1.00	13.83
ATOM	2341	CD2	TRP	A1075	58.962	64.566	36.350	1.00	13.83
ATOM	2342	NE1	TRP	A1075	59.683	64.256	34.259	1.00	13.83
ATOM	2343	CE2	TRP	A1075	58.593	64.109	35.078	1.00	13.83
ATOM	2344	CE3	TRP	A1075	58.029	64.518	37.373	1.00	13.83
ATOM	2345	CZ2		A1075	57.303	63.604	34.801	1.00	
ATOM	2346	CZ3	TRP		56.751	64.011	37.074	1.00	13.83
ATOM	2347	CH2	TRP		56.423	63.573	35.814	1.00	13.83
ATOM	2350	N		A1076	63.867	65.842	39.597		
ATOM	2351	CA		A1076	64.354	66.722		1.00	99.49
ATOM	2352	C		A1076	64.967		40.635	1.00	99.49
ATOM	2353	0		A1076		67.872	39.838	1.00	99.49
ATOM	2354	CB			65.185	67.747	38.637	1.00	
ATOM	2355			A1076	65.412	66.011	41.484		96.28
ATOM	2355	CG		A1076	64.948	64.665	42.026		96.28
		CD		A1076	65.966	64.028	42.968		96.28
ATOM	2357	NE		A1076	65.361	63.411	44.155	1.00	
ATOM	2358	CZ		A1076	65.408	62.110	44.427		96.28
ATOM	2359	NH1		A1076	66.029	61.286	43.595		96.28
ATOM	2360	NH2		A1076	64.855	61.635	45.538		96.28
ATOM	2367	N		A1077	65.200	69.008	40.469		54.46
ATOM	2368	CA		A1077	65.824	70.107	39.764	1.00	54.46
ATOM	2369	C	GLU	A1077	67.293	69.771	39.587	1.00	54.46

. FIG. 6HH

ATOM	2370	0	GLU	J A1077	67.7	27 69.428	38.509	1.00 54.46
ATOM	2371	CB	GLU	J A1077	65.6			1.00 10.55
ATOM	2373	N		A1078	68.0			1.00 35.40
ATOM	2374	CA		A1078	69.4			1.00 35.40
ATOM	2375	C		A1078	69.7			1.00 35.40
ATOM	2376	0	LYS		69.59			1.00 35.40
ATOM	2377	CB	LYS	A1078	69.99			1.00 35.40
ATOM	2378	CG	LYS		70.05			1.00 95.51
ATOM	2379	CD	LYS	A1078	70.00			1.00 95.51
ATOM	2380	CE	LYS		71.48			1.00 95.51
ATOM	2381	NZ	LYS	A1078	71.57			1.00 95.51
ATOM	2386	N	PRO	A1079	70.23			1.00 54.45
MOTA	2387	CA	PRO	A1079	70.43			1.00 54.45
MOTA	2388	C	PRO	A1079	71.17			1.00 54.45
ATOM	2389	0	PRO	A1079	70.74		38.040	1.00 54.45
ATOM	2390	CB	PRO	A1079	71.09		36.381	1.00 46.70
ATOM	2391	CG	PRO	A1079	70.73		36.376	1.00 46.70
ATOM	2392	CD	PRO	A1079	70.65		37.801	1.00 46.70
ATOM	2393	N	TYR	A1080	72.26		38.968	1.00100.00
ATOM	2394	CA	TYR	A1080	72.96		39.542	1.00100.00
ATOM	2395	C	TYR	A1080	72.12		40.621	1.00100.00
ATOM	2396	0	TYR	A1080	72.61		41.375	1.00100.00
ATOM	2397	CB	TYR	A1080	74.30		40.141	1.00 41.54
ATOM	2398	CG	TYR	A1080	74.19		40.985	1.00 41.54
ATOM	2399	CD1	TYR	A1080	73.91	2 66.774	42.320	1.00 41.54
ATOM	2400	CD2	TYR	A1080	74.31		40.422	1.00 41.54
ATOM	2401	CE1	TYR	A1080	73.75		43.061	1.00 41.54
ATOM	2402	CE2	TYR	A1080	74.15	8 69.220	41.161	1.00 41.54
ATOM	2403	CZ		A1080	73.88	2 69.118	42.480	1.00 41.54
ATOM	2404	OH	TYR	A1080	73.77	8 70.273	43.233	1.00 41.54
ATOM	2407	N		A1081	70.87	0 64.982	40.712	1.00 38.29
ATOM	2408	CA		A1081	69.94	8 64.379	41.652	1.00 38.29
MOTA	2409	C		A1081	59.03	0 63.423	40.853	1.00 38.29
ATOM	2410	0		A1081	68.52	2 62.448	41.398	1.00 38.29
MOTA	2411	CB		A1081	69.21	4 65.451	42.451	1.00 37.33
ATOM	2412	CG		A1081	69.92	7 65.679	43.797	1.00 37.33
ATOM	2413	CD		A1081	69.52		44.542	1.00 37.33
ATOM	2414			A1081	70.08		45.646	1.00 37.33
MOTA	2415			A1081	68.67		44.045	1.00 37.33
ATOM	2417	N		A1082	68.87		39.550	1.00 35.27
ATOM	2418	CA		A1082	68.15		38.655	1.00 35.27
ATOM	2419	C		A1082	68.83		38.883	1.00 35.27
ATOM	2420	0		A1082	69.93		39.463	1.00 35.27
ATOM ATOM	2421	CB		A1082	68.33		37.216	1.00 62.49
	2422	CG		A1082	67.20		36.647	1.00 62.49
ATOM ATOM	2423	CD		A1082	67.29		36.942	1.00 62.49
ATOM	2424	NE		A1082	67.44		35.737	1.00 62.49
ATOM		CZ		A1082	67.099		35.661	1.00 62.49
ATOM	2426			A1082	66.58		36.705	1.00 62.49
ATOM	2434	NH2 N		A1082	67.31		34.547	1.00 62.49
ATOM	2435		PRO	A1083	68.144		38.530	1.00 37.62
ATOM	2435	CA C		A1083	68.732		38.729	1.00 37.62
ATOM	2435	0		A1083	69.270		37.461	1.00 37.62
ATOM	2437	CB		A1083	68.905		36.414	1.00 37.62
ATOM	2438	CG		A1083 A1083	67.541		39.267	1.00 40.57
ATOM	2440	CD		A1083	66.294		39.213	1.00 40.57
	-770	CD	210	MIU83	66.72	L 60.125	38.171	1.00 40.57

FIG. 6II

MOTA

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ATOM	2441	N	SED	A1084	70.157	57.337	37.541	1.00 23.77
ATOM	2442	CA		A1084	70.642	56.597	36.339	1.00 23.77
ATOM	2443	C		A1084	69.465	55.689	35.826	1.00 23.77
ATOM	2444	0		A1084	68.690	55.172	36.633	1.00 23.77
ATOM	2445	CB		A1084	71.772	55.617	36.733	1.00 23.77
ATOM	2445	OG		A1084	71.518	55.019	38.069	1.00 2.00
ATOM	2449	N		A1084	69.330	55.466	34.520	1.00 44.36
ATOM	2450	CA		A1085	68.272	54.565	34.032	1.00 44.36
ATOM	2451	C		A1085			34.801	1.00 44.36
ATOM	2451	0		A1085	68.458	53.237	35.603	1.00 44.36
ATOM	2453	CB		A1085	67.633	52.852 54.399	32.529	1.00 44.36
ATOM	2454	CG		A1085	68.414 68.175	55.669	31.783	1.00 95.75
ATOM	2455	CD1		A1085			30.866	1.00 95.75
ATOM	2455	CD2		A1085	69.088	56.137		
ATOM	2457	CE1		A1085	67.036	56.409	32.022	1.00 95.75 1.00 95.75
ATOM	2457	CE2		A1085	68.863	57.321 57.591	31.361	1.00 95.75
ATOM	2459	CZ			66.807		30.452	1.00 95.75
ATOM	2461	N		A1085	67.713	58.049	34.541	
				A1086	69.541	52.541		1.00 35.91
ATOM ATOM	2462	CA C		A1086	69.894	51.395	35.347	1.00 35.91
	2463			A1086	69.171	51.316	36.743	1.00 35.91
ATOM	2464	0		A1086	68.741	50.223	37.179	1.00 35.91
MOTA	2465	CB		A1086	71.400	51.423	35.580	1.00 44.62
MOTA	2467	N		A1087	69.081	52.427	37.464	1.00 20.15
ATOM	2468	CA		A1087	68.394	52.412	38.732	1.00 20.15
ATOM	2469	С		A1087	66.842	52.338	38.466	1.00 20.15
ATOM	2470	0		A1087	66.039	51.538	39.059	1.00 20.15
ATOM	2471	CB		A1087	68.766	53.690	39.501	1.00 19.20
MOTA	2472	CG		A1087	70.227	53.686	40.069	1.00 19.20
ATOM	2473	CD		A1087	70.563	54.908	40.926	1.00 19.20
ATOM	2474	OE1		A1087	70.927	55.939	40.379	1.00 19.20
ATOM	2475	NE2		A1087	70.473	54.783	42.263	1.00 19.20
ATOM	2479	N		A1088	66.451	53.197	37.550	1.00 25.82
ATOM	2480	CA		A1088	65.088	53.310	37.160	1.00 25.82
MOTA	2481	C		A1088	64.852	51.851	36.847	1.00 25.82
ATOM	2482	0		A1088	63.966	51.300	37.447	1.00 25.82
ATOM	2483	CB		A1088	64.921	54.260	35.919	1.00 17.84
ATOM	2484	CG1		A1088	65.069	55.704	36.340	1.00 17.84
ATOM	2485	CG2 CD1		A1088	63.626	53.984	35.170	1.00 17.84
ATOM ATOM	2486			A1088	65.738	56.545	35.203	1.00 17.84
	2488	N		A1089	65.628	51.205	35.969	1.00 19.62
ATOM	2489	CA		A1089	65.380	49.747	35.692	1.00 19.62
ATOM	2490	C		A1089	65.471	48.746	36.793	1.00 19.62
MOTA	2491	0		A1089	64.899	47.746	36.680	1.00 19.62
ATOM	2492	CB		A1089	66.155	49.127	34.566	1.00 2.73
ATOM	2493	CG		A1089	65.363	47.882	33.978	1.00 2.73
MOTA	2494	CD1		A1089	65.305	47.787	32.425	1.00 2.73
ATOM	2495	CD2		A1089	66.127	46.642	34.338	1.00 2.73
ATOM	2497	N		A1090	66.164	48.988	37.866	1.00 15.82
ATOM	2498	CA		A1090	66.074	47.993	38.898	1.00 15.82
ATOM	2499	C		A1090	64.931	48.400	39.791	1.00 15.82
ATOM	2500	0		A1090	64.700	47.776	40.834	1.00 15.82
ATOM	2501	CB		A1090	67.396	47.811	39.695	1.00 8.61
ATOM	2502	CG1		A1090	67.259	48.053	41.220	1.00 8.61
ATOM	2503	CG2		A1090	67.829	46.397	39.452	1.00 8.61
ATOM ATOM	2505 2506	N CA		A1091	64.218	49.451	39.377	1.00 45.24
ATOM	2506	CM	SER	A1091	63.073	50.005	40.110	1.00 45.24

61.708 49.486 39.628 1.00 45.24

ATOM	2508	0	SEP	A1091	60.764	49.305	40.422	1.00 45.24
ATOM	2509	CB		A1091	63.064	51.511	39.963	1.00 46.04
ATOM	2510	OG		A1091	62.473	52.119	41.083	1.00 46.04
ATOM	2513	N		A1092	61.582	49.317	38.318	1.00 48.10
ATOM	2514	CA		A1092	60.336	48.814	37.772	1.00 48.10
ATOM	2515	C		A1092	60.362	47.286	37.896	1.00 48.10
ATOM	2516	0		A1092	59.310	46.649	38.093	1.00 48.10
MOTA	2517	CB		A1092	60.226	49.217	36.335	1.00 20.50
ATOM	2518	CG		A1092	60.649	50.636	36.171	1.00 20.50
ATOM	2519	CD1		A1092	61.112	50.957	34.819	1.00 20.50
ATOM	2520			A1092	59.492	51.389	36.445	1.00 20.50
ATOM	2522	N		A1093	61.588	46.721	37.764	1.00 21.90
ATOM	2523	CA		A1093	61.816	45.284	37.914	1.00 21.90
ATOM	2524	C	ASN	A1093	61.298	44.970	39.321	1.00 21.90
ATOM	2525	0	ASN	A1093	60.506	44.064	39.515	1.00 21.90
ATOM	2526	CB	ASN	A1093	63.301	45.010	37.802	1.00 40.34
ATOM	2527	CG	ASN	A1093	63.756	44.903	36.364	1.00 40.34
ATOM	2528	OD1	ASN	A1093	64.796	44.322	36.103	1.00 40.34
ATOM	2529	ND2	ASN	A1093	62.989	45.468	35.422	1.00 40.34
ATOM	2533	N		A1094	61.699	45.746	40.314	1.00 34.76
ATOM	2534	CA		A1094	61.194	45.385	41.611	1.00 34.76
ATOM	2535	C		A1094	59.685	45.221	41.451	1.00 34.76
ATOM	2536	ō		A1094	59.122	44.320	42.022	1.00 34.76
ATOM	2537	CB		A1094	61.515	46.451	42.653	1.00 99.74
ATOM	2538	CG		A1094 A1094	61.377	45.969	44.088	1.00 99.74
ATOM	2539	CD						
ATOM		NE		A1094	59.934	46.037	44.575	1.00 99.74
ATOM	2540			A1094	59.736	47.099	45.557	1.00 99.74
	2541	CZ		A1094	58.550	47.590	45.907	1.00 99.74
ATOM	2542			A1094	57.438	47.117	45.357	1.00 99.74
MOTA	2543	NH2		A1094	58.479	48.565	46.805	1.00 99.74
ATOM	2550	M		A1095	59.045	46.073	40.640	1.00 52.46
MOTA	2551	CA		A1095	57.594	46.029	40.452	1.00 52.46
MOTA	2552	C		A1095	57.136	44.721	39.781	1.00 52.46
ATOM	2553	0		A1095	56.663	43.809	40.435	1.00 52.46
ATOM	2554	CB		A1095	57.151	47.287	39.683	1.00 62.45
ATOM	2555	CG		A1095	57.076	48.578	40.594	1.00 62.45
MOTA	2556	SD	MET	A1095	57.031	50.297	39.847	1.00 62.45
ATOM	2557	CE	MET	A1095	57.509	51.299	41.162	1.00 62.45
ATOM	2559	N	LEU	A1096	57.289	44.666	38.476	1.00 14.04
ATOM	2560	CA.	LEU	A1096	57.029	43.531	37.600	1.00 14.04
ATOM	2561	C	LEU	A1096	57.039	42.101	38.255	1.00 14.04
ATOM	2562	0	LEU	A1096	56.575	41.148	37.638	1.00 14.04
ATOM	2563	CB	LEU	A1096	58.046	43.560	36.441	1.00 37.25
ATOM	2564	CG	LEU	A1096	58.047	44.610	35.300	1.00 37.25
ATOM	2565			A1096	59.158	44.291	34.269	1.00 37.25
ATOM	2566	CD2		A1096	56.643	44.684	34.592	1.00 37.25
ATOM	2568	N		A1097	57.574	41.928	39.450	1.00 42.58
ATOM	2569	CA		A1097	57.530	40.621	40.048	1.00 42.58
ATOM	2570	C		A1097	56.651	40.621	41.296	1.00 42.58
ATOM	2571	0		A1097	57.019	40.890	42.411	1.00 42.58
ATOM	2572	CB		A1097			40.396	1.00100.00
					58.919	40.136		
ATOM	2573	CG		A1097	59.757	39.901	39.188	1.00100.00
ATOM	2574	CD		A1097	60.925	40.839	39.144	1.00100.00
MOTA	2575	OE1		A1097	61.083	41.611	40.117	1.00100.00
MOTA	2576	OE2		A1097	61.680	40.799	38.147	1.00100.00
MOTA	2578	N		A1098	55.454	41.211	41.108	1.00 43.50
ATOM	2579	CA	GLU	A1098	54.540	41.313	42.226	1.00 43.50

ATOM	2580	С	GL	U A1098	53.112	41.239	41.679	1.00 43.50
ATOM	2581	0	GL	J A1098	52.247	40.533	42.228	
ATOM	2582	CB		J A1098	54.783	42.639	42.220	1.00 43.50
ATOM	2583	CG		J A1098	56.233			1.00 60.12
ATOM	2584	CD		J A1098	56.895	43.014	43.093	1.00 60.12
ATOM	2585	OE:		J A1098		42.498	44.392	1.00 60.12
ATOM	2586	OE		J A1098	56.253	42.586	45.481	1.00 60.12
ATOM	2588	N N			58.071	42.019	44.331	1.00 60.12
ATOM	2589	CA		A1099	52.896	41.931	40.566	1.00100.00
ATOM	2590			A1099	51.564	42.010	40.005	1.00100.00
ATOM	2590	0		A1099	50.792	42.471	41.232	1.00100.00
		_		A1099	50.117	41.681	41.899	1.00100.00
ATOM	2592	CB		A1099	51.050	40.643	39.530	1.00 69.49
ATOM	2593	CG		A1099	49.707	40.745	38.761	1.00 69.49
ATOM	2594	CD		A1099	49.883	40.941	37.244	1.00 69.49
ATOM	2595	NE		A1099	49.647	42.326	36.812	1.00 69.49
MOTA	2596	CZ		A1099	49.095	42.672	35.648	1.00 69.49
ATOM	2597	NH1		A1099	48.705	41.740	34.782	1.00 69.49
ATOM	2598	NH2	ARC	A1099	48.989	43.951	35,322	1.00 69.49
MOTA	2605	N	LYS	A1100	50.957	43.748	41.555	1.00 49.25
ATOM	2606	CA	LYS	A1100	50.308	44.328	42,698	1.00 49.25
ATOM	2607	C	LYS	A1100	49.232	45.070	42.019	1.00 49.25
MOTA	2608	0	LYS	A1100	48.111	45.129	42.502	1.00 49.25
ATOM	2609	CB	LYS	A1100	51.247	45.296	43.419	1.00 99.82
ATOM	2610	CG	LYS	A1100	50.853	45.635	44.859	1.00 99.82
ATOM	2611	CD	LYS		50.997	44.447	45.815	1.00 99.82
ATOM	2612	CE	LYS	A1100	49.635	43.868	46.212	1.00 99.82
ATOM	2613	NZ		A1100	49.247	44.148	47.622	1.00 99.82
ATOM	2618	N		A1101	49.603	45.578	40.850	1.00 99.82
AT'OM	2619	CA		A1101	48.769	46.370	39.946	
ATOM	2620	C		A1101	49.030	47.835		1.00 64.74
ATOM	2621	ō		A1101	48.381	48.463	40.194 41.014	1.00 64.74
ATOM	2622	CB		A1101	47.282			1.00 64.74
ATOM	2623	0G1		A1101	47.282	46.080	40.069	1.00100.00
ATOM	2624	CG2		A1101	46.581	44.676	40.244	1.00100.00
ATOM	2627	N		A1101		46.494	38.801	1.00100.00
ATOM	2628	CA		A1102	50.026	48.346	39.472	1.00 78.61
ATOM	2629	C		A1102 A1102	50.462	49.715	39.571	1.00 78.61
ATOM	2630	0			49.666	50.619	38.672	1.00 78.61
ATOM	2631	CB		A1102	49.438	51.753	39.026	1.00 78.61
ATOM	2632	CG		A1102	51.960	49.856	39.210	1.00 42.69
ATOM	2633			A1102	52.910	49.107	40.092	1.00 42.69
ATOM		CD1		A1102	53.228	47.735	39.812	1.00 42.69
ATOM	2634 2635	CD2		A1102	53.356	49.663	41.288	1.00 42.69
		CEl		A1102	53.926	46.943	40.711	1.00 42.69
ATOM	2636	CE2		A1102	54.061	48.880	42.207	1.00 42.69
MOTA	2637	CZ		A1102	54.327	47.512	41.917	1.00 42.69
ATOM	2638	OH		A1102	54.871	46.698	42.873	1.00 42.69
ATOM	2641	N		A1103	49.233	50.151	37.513	1.00100.00
ATOM	2642	CA		A1103	48.509	51.066	36.650	1.00100.00
ATOM	2643	C		A1103	47.068	50.762	36.293	1.00100.00
MOTA	2644	0		A1103	46.757	50.368	35.175	1.00100.00
MOTA	2645	CB		A1103	49.276	51.326	35.350	1.00100.00
ATOM	2646	CG1	VAL	A1103	48.590	52.426	34.565	1.00100.00
MOTA	2647	CG2	VAL	A1103	50.694	51.746	35.661	1.00100.00
ATOM	2649	N	ASN	A1104	46.191	50.990	37.260	1.00 30.52
MOTA	2650	CA	ASN	A1104	44.768	50.802	37.118	1.00 30.52
ATOM	2651	С		A1104	44.245	51.216	35.761	1.00 30.52
ATOM	2652	0		A1104	44.475	52.317	35.289	1.00 30.52
							- 3 . 20 3	2.30 30.32

2663 0

2669 N

ATOM

ATOM

ATOM

ATOM ATOM THR A1105

THR A1105

THR A1106

2664 CB THR A1105

2665 OG1 THR A1105 2666 CG2 THR A1105 44.041 51.572 38.171 1.00 63.62 42.646 51.154 38.272 1.00 63.62 41.934 51.137 37.275 1.00 63.62

1.00 63.62

42.224 50.788 39.469

ATOM 2670 CA THR A1106 ATOM 2671 C THR A1106 ATOM 2672 0 THR A1106 ATOM 2673 CB THR A1106 ATOM 2674 OG1 THR A1106 ATOM 2675 CG2 THR Al106 ATOM 2678 N LEU Allo7 ATOM 2679 CA LEU Al107 Ö ATOM 2680 C LEU All07 ATOM 2681 0 LEU Allo7 10 2682 CB LEU Al107 ATOM 14 ATOM 2683 CG LEU All07 ATOM 2684 CD1 LEU All07 ATOM 2685 CD2 LEU All07 ATOM 2687 N TYR All08 ATOM 2688 CA TYR A1108 bet. 2689 C TYR A1108 ATOM ATOM 2690 O TYR A1108 2691 CB TYR A1108 ATOM 111 ATOM 2692 CG TYR A1108 tu ATOM 2693 CD1 TYR All08 fij ATOM 2694 CD2 TYR A1108 O ATOM 2696 N GLU A1109 2697 CA GLU A1109 Lat. ATOM 2698 C GLU All09 ATOM ATOM 2699 0 GLU A1109 ATOM 2700 CB GLU A1109 ATOM 2702 N LYS A1110 2703 CA LYS A1110 ATOM ATOM 2704 C LYS A1110 2705 O ATOM LYS A1110 ATOM 2706 CB LYS A1110 ATOM 2707 CG LYS A1110 ATOM 2708 CD LYS A1110 ATOM 2709 CE LYS A1110 ATOM 2710 NZ LYS A1110 ATOM 2715 N PHE A1111 2716 CA PHE A1111 ATOM

2717 C

2718 0

2719 CB

PHE Alli

PHE Alli

PHE Allil

2720 CG PHE A1111

2721 CD1 PHE A1111

2722 CD2 PHE A1111 2723 CE1 PHE A1111

ATOM

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ATOM

43.519 50.305 35.135 1.00 45.33 42.978 50.501 33.817 1.00 45.33 41.629 49.788 33.751 1.00 45.33 1.00 45.33 40.980 49.726 32.734 43.987 49.959 32.817 1.00 46.03 44.604 48.759 33.328 1.00 46.03 45.083 50.972 32.633 1.00 46.03 41.199 49.243 34.869 1.00 15.59 39.900 48.589 34.956 1.00 15.59 38.820 49.661 35.289 1.00 15.59 39.072 50.461 36.167 1.00 15.59 39.931 47.514 36.091 1.00 59.09 39.776 46.205 35.525 1.00 59.09 38.827 47.743 37.083 1.00 59.09 37.641 49.683 34.662 1.00 27.67 36.613 50.729 35.028 1.00 27.67 35.966 50.401 36.392 1.00 27.67 34.939 49.735 36.477 1.00 27.67 35.491 50.874 33.967 1.00 39.85 35.834 50.768 32.492 1.00 39.85 34.611 50.486 31.731 1.00 39.85 36.500 51.981 31.985 1.00 39.85 36.576 50.816 37.480 1.00 99.39 35.969 50.482 38.748 1.00 99.39 34.685 51.305 38.878 1.00 99.39 33.900 51.097 39.806 1.00 99.39 36.973 50.749 39.872 1.00100.00 38.383 50.249 39.513 1.00100.00 39.286 51.419 39.214 1.00100.00 38.945 49.421 40.644 1.00100.00 34.486 52.198 37.899 1.00100.00 33.341 53.116 37.779 1.00100.00 33.875 54.536 37.598 1.00100.C0 34.957 54.846 38.095 1.00100.00 32.454 53.065 39.001 1.00 76.82 33.104 55.390 36.914 1.00100.00 33,486 56,779 36,626 1,00100.00 34.891 56.830 36.038 1.00100.00 35.858 56.673 36.763 1.00100.00 33.430 57.631 37.900 1.00 99.15 34.009 56.977 39.152 1.00 99.15 34.718 57.970 40.052 1.00 99.15 34.246 57.852 41.490 1.00 99.15 33.479 59.054 41.919 1.00 99.15 35.030 57.055 34.737 1.00100.00 36.373 57.068 34.186 1.00100.00 36.824 58.244 33.333 1.00100.00 36.116 58.763 32.487 1.00100.00

39.101

*36.685 55.747 33.449

55.397 34.055 38.575 55.820 31.785

40.448 55.431 33.736 1.00 61.16

38.144 55.601 33.081

1.00 61.16

1.00 61.16

1.00 61.16

1.00 61.16

ATOM	2724	CE2	PHE	A1111	39.917	55.853	31.485	1.00	61.16
ATOM	2725	CZ		A1111	40.845	55.664	32.451		61.16
ATOM	2727	N		A1112	38.080	58.579	33.586		54.03
ATOM	2728	CA		A1112	38.875	59.664	33.030		54.03
ATOM	2729	C		A1112	39.433	59.610	31.628		54.03
ATOM	2730	0		A1112	38.693	59.607	30.694		54.03
ATOM	2731	CB		A1112	40.029	59.942	34.007		.00.00
ATOM	2732	OG1		A1112	41.181	59.195	33.618		.00.00
ATOM	2733	CG2		A1112	39.637	59.498	35.430		.00.00
ATOM	2736	N		A1113	40.750	59.639	31.504		39.45
ATOM	2737	CA		A1113	41.514	59.623	30.240		39.45
ATOM	2738	C		A1113	42.391	60.886	30.057		39.45
ATOM	2739	ō		A1113	42.658	61.611	30.980		39.45
ATOM	2740	CB		A1113	40.661	59.461	29.000		60.42
ATOM	2741	CG		A1113	40.682	58.097	28.373		60.42
ATOM	2742	CD1		A1113	40.002	57.867	27.193		60.42
ATOM	2743	CD2		A1113	41.168	56.982	29.056		60.42
ATOM	2744	CE1		A1113	39.776	56.585	26.720		60.42
ATOM	2745	CE2		A1113	40.938	55.670	28.577		60.42
ATOM	2746	CZ		A1113	40.930	55.511	27.413		60.42
ATOM	2747	OH		A1113					
					39.943	54.290	26.912		60.42
ATOM	2750	N		A1114	42.852	61.153	28.847		.00.00
ATOM	2751	CA		A1114	43.759	62.268	28.741		.00.00
MOTA	2752	C		A1114	44.080	62.762	27.312		.00.00
ATOM	2753	0		A1114	44.093	63.971	27.052		.00.00
MOTA	2754	CB		A1114	45.049	61.857	29.500		34.32
ATOM	2756	N		A1115	44.317	61.803	26.410		68.47
MOTA	2757	CA		A1115	44.683	62.024	24.996		68.47
ATOM	2758	C		A1115	44.399	63.213	24.093		68.47
ATOM	2759	0		A1115	45.017	63.303	23.036		68.47
MOTA	2761	N		A1116	43.470	64.088	24.487		.00.00
ATOM	2762	CA		A1116	43.066	65.299	23.739		.00.00
ATOM	2763	C		A1116	41.700	65.193	23.039		.00.00
ATOM	2764	0		A1116	41.049	64.140	23.163		.00.00
ATOM	2765	CB		A1116	44.141	65.709	22.727		87.32
MOTA	2766	OXT	ILE	A1116	41.280	66.178	22.385	1.00	87.32
TER									
HETATM	1	C1	INH	I 1	58.113	50.247	12.231	0.00	0.00
HETATM	2	N2	INH	1 1	57.524	51.444	12.292	0.00	0.00
HETATM	3	C3	INH	I 1	58.303	52.541	12.107	0.00	0.00
HETATM	4	C4	INH	I 1	59.686	52.462	12.036	0.00	0.00
HETATM	5	C5	INH	I 1	60.234	51.117	12.080	0.00	0.00
HETATM	6	N6	INH	I 1	59.434	50.040	12.174	0.00	0.00
HETATM	8	N8	INH	I 1	57.877	53.857	12.079	0.00	0.00
HETATM	9	C9	INH	I 1	59.057	54.550	11.988	0.00	0.00
HETATM	10	C10	INH	I 1	60.219	53.760	11.953	0.00	0.00
HETATM	12	C13	INH	I 1	61.633	54.217	11.871	0.00	0.00
HETATM	13	N15	INH	I 1	61.632	50.906	12.042	0.00	0.00
HETATM	14	C16	INH	I 1	56.477	54.327	12.146	0.00	0.00
HETATM	15	C17	INH	I 1	56.258	55.192	13.391	0.00	0.00
HETATM	16	C18	INH	I 1	54.809	55.688	13.471	0.00	0.00
HETATM	17	C19	INH	I 1	54.371	56.477	12.214	0.00	0.00
HETATM	18	C20	INH	I 1	54.670	55.630	10.955	0.00	0.00
HETATM	19	C21	INH	I 1	56.121	55.136	10.897	0.00	0.00
HETATM	28	N30	INH		52.949	56.902	12.268	0.00	0.00
HETATM	29	C32	INH	I 1	51.997	55.774	12.311	0.00	0.00
HETATM	30	C33	INH	I 1	50.531	56.215	12.400	0.00	0.00

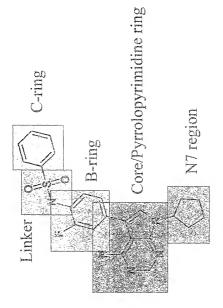
Docket/App No.: 2079.1037-001

Title: Method of Identifying Inhibitors of TIE-2

Nancy J. Bump et al. Inventors:

Kinase catalytic domain structure walkthrough - insulin receptor kinase Side nucleotide binding loop activation loop catalytic loop ATP/Mg substrare Front

DOGGETHER - DIFFE



Inhibitor I structural elements

BSF421386 binding region

hinge
purine core
extended sugar
y plumphate
nucleotide binding
early activation loop
catalytic lysine
distal hydrophobic
miscellaneous

